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(54) Title: A METHOD OF DESIGNING ALPHA-AMYLASE MUTANTS WITH PREDETERMINED PROPERTIES (57) Abstract A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least one altered property as compared to the parent α -amylase, comprises i) analysing the structure of the parent Termamyl-like α -amylase to identify at least one amino acid residue or at least one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is believed to be of relevance for altering the property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations), ii) constructing a Termamyl-like α -amylase variant, which as compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter the property, and iii) testing the resulting Termamyl-like α -amylase variant for the property in question.		

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A METHOD OF DESIGNING ALPHA-AMYLASE MUTANTS WITH PREDETERMINED PROPERTIES

FIELD OF THE INVENTION

5 The present invention relates to a novel method of designing α -amylase mutants with predetermined properties, which method is based on the hitherto unknown three-dimensional structure of bacterial α -amylases.

10 BACKGROUND OF THE INVENTION

α -Amylases (α -1,4 glucan-4-glucanohydrolase, EC 3.2.1.1) constitute a group of enzymes which is capable of hydrolyzing starch and other linear and branched 1,4-glucosidic oligo- and
15 polysaccharides. Almost all α -amylases studied have a few conserved regions with approximately the same length and spacing. One of these regions resembles the Ca^{2+} binding site of calmodulin and the others are thought to be necessary for the active centre and/or binding of the substrate.

20

While the amino acid sequence and thus primary structure of a large number of α -amylases are known, it has proved very difficult to determine the three-dimensional structure of all α -amylases. The three-dimensional structure can be determined
25 by X-ray crystallographic analysis of α -amylase crystals, but it has proven difficult to obtain α -amylase crystals suitable for actually solving the structure.

Until now the three-dimensional structure of only a few
30 α -amylases have been determined at high resolution. These include the structure of the *Aspergillus oryzae* TAKA α -amylase (Swift et al., 1991), the *Aspergillus niger* acid amylase (Brady et al, 1991), the structure of pig pancreatic α -amylase (Qian et al., 1993), and the barley alpha-amylase (Kadziola et al.
35 1994, Journal of Molecular Biology 239: 104-121, A.Kadziola, Thesis, Dept of Chemistry, U. of Copenhagen, Denmark). Furthermore, the three-dimensional structure of a *Bacillus circulans* cyclodextrin glycosyltransferase (CGTase) is known

(Klein et al., 1992) (Lawson et al., 1994). The CGTase catalyzes the same type of reactions as α -amylases and exhibits some structural resemblance with α -amylases.

5 Furthermore, crystallization and preliminary X-ray studies of *B. subtilis* α -amylases have been described (Chang et al. (1992) and Mizuno et al. (1993)). No final *B. subtilis* structure has been reported. Analogously, the preparation of *B. licheniformis* α -amylase crystals has been reported (Suzuki et al. (1990)), but
10 no subsequent report on X-ray crystallographic analysis or three-dimensional structure are available.

Several research teams have attempted to build three-dimensional structures on the basis of the above known
15 α -amylase structures. For instance, Vihinen et al. (J. Biochem. 107, 267-272, 1990), disclose the modelling (or computer simulation) of a three-dimensional structure of the *Bacillus stearothermophilus* α -amylase on the basis of the TAKA amylase structure. The model was used to investigate hypothetical
20 structural consequences of various site-directed mutations of the *B. stearothermophilus* α -amylase. E.A. MacGregor (1987) predicts the presence of α -helices and β -barrels in α -amylases from different sources, including barley, pig pancreas and *Bacillus amyloliquefaciens* on the basis of the known structure
25 of the *A. oryzae* TAKA α -amylase and secondary structure predicting algorithms. Furthermore, the possible loops and subsites which may be found to be present in, e.g., the *B. amyloliquefaciens* α -amylase are predicted (based on a comparison with the *A. oryzae* sequence and structure).

30

A.E. MacGregor (Starch/Stärke 45 (1993), No. 7, p. 232-237) presents a review of the relationship between the structure and activity of α -amylase related enzymes.

35 Hitherto, no three-dimensional structure has been available for the industrially important *Bacillus* α -amylases (which in the present context are termed "Termamyl-like α -amylases"),

including the *B. licheniformis*, the *B. amyloliquefaciens*, and the *B. stearothermophilus* α -amylase.

BRIEF DISCLOSURE OF THE INVENTION

5

The three-dimensional structure of a Termamyl-like bacterial α -amylase has now been elucidated. On the basis of an analysis of said structure it is possible to identify structural parts or specific amino acid residues which from structural or
10 functional considerations appear to be important for conferring the various properties to the Termamyl-like α -amylases. Furthermore, when comparing the Termamyl-like α -amylase structure with known structures of the fungal and mammalian α -amylases mentioned above, it has been found that some
15 similarities exist between the structures, but also that some striking, and not previously predicted structural differences between the α -amylases exist. The present invention is based on these findings.

20 Accordingly, in a first aspect the invention relates to a method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least one altered property as compared to said parent α -amylase, which method comprises

25

i) analysing the structure of the Termamyl-like α -amylase with a view to identifying at least one amino acid residue or at least one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is
30 believed to be of relevance for altering said property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations),

ii) constructing a Termamyl-like α -amylase variant, which as
35 compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

iii) testing the resulting Termamyl-like α -amylase variant for said property.

- 5 In a second aspect the present invention relates to a method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method comprises
- 10 i) comparing the three-dimensional structure of the Termamyl-like α -amylase with the structure of a non-Termamyl-like α -amylase,
- ii) identifying a part of the Termamyl-like α -amylase structure which is different from the non-Termamyl-like α -amylase
- 15 structure, and
- iii) modifying the part of the Termamyl-like α -amylase identified in ii) whereby a Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α -amylase.

20

In a third aspect the invention relates to a method of constructing a variant of a parent non-Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method

25 comprises

- i) comparing the three-dimensional structure of the non-Termamyl-like α -amylase with the structure of a Termamyl-like α -amylase,
- ii) identifying a part of the non-Termamyl-like α -amylase
- 30 structure which is different from the Termamyl-like α -amylase structure, and
- iii) modifying the part of the non-Termamyl-like α -amylase identified in ii) whereby a non-Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the
- 35 parent Termamyl-like α -amylase.

The property which may be altered by the above methods of the present invention may, e.g., be substrate specificity,

substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6, in particular pH<5) or high (e.g. pH>9) pH values), stability
5 towards oxidation, Ca²⁺-dependency, specific activity, and other properties of interest. For instance, the alteration may result in a variant which, as compared to the parent Termamyl-like α -amylase, has an increased specific activity at a given pH and/or an altered substrate specificity.

10

In still further aspects the invention relates to variants of a Termamyl-like α -amylase, DNA encoding such variants and methods of preparing the variants. Finally, the invention relates to the use of the variants for various industrial
15 purposes.

DETAILED DISCLOSURE OF THE INVENTION

The Termamyl-like α -amylase

20

It is well known that a number of alpha-amylases produced by *Bacillus* spp. are highly homologous on the amino acid level. For instance, the *B. licheniformis* α -amylase comprising the amino acid sequence shown in SEQ ID No. 2 (commercially
25 available as Termamyl®) has been found to be about 89% homologous with the *B. amyloliquefaciens* α -amylase comprising the amino acid sequence shown in SEQ ID No. 4 and about 79% homologous with the *B. stearothermophilus* α -amylase comprising the amino acid sequence shown in SEQ ID No. 6. Further
30 homologous α -amylases include an α -amylase derived from a strain of the *Bacillus* sp. NCIB 12289, NCIB 12512, NCIB 12513 or DSM 9375, all of which are described in detail in WO 95/26397, and the α -amylase described by Tsukamoto et al., 1988, Biochemical and Biophysical Research Communications, Vol.
35 151, No. 1. Still other homologous α -amylases include the α -amylase produced by the *B. licheniformis* described in EP 252 666 (ATCC 27811), and the α -amylases identified in WO 91/00353 and WO 94/18314. Other commercial Termamyl-like E.

licheniformis α -amylases are Optitherm[®] and Takatherm[®] (available from Solvay), Maxamyl[®] (available from Gist-brocades/Genencor), Spezym AA[®] (available from Genencor), and Keistase[®] (available from Daiwa).

5

Because of the substantial homology found between these α -amylases, they are considered to belong to the same class of α -amylases, namely the class of "Termamyl-like α -amylases".

- 10 Accordingly, in the present context, the term "Termamyl-like α -amylase" is intended to indicate an α -amylase which, on the amino acid level, exhibits a substantial homology to Termamyl[®], i.e. the *B. licheniformis* α -amylase SEQ ID NO 2. In other words, a Termamyl-like α -amylase is an α -amylase, which has the
- 15 amino acid sequence shown in SEQ ID No. 2, 4 or 6 herein, or the amino acid sequence shown in SEQ ID NO 1 or 2 of WO 95/26397 or in Tsukamoto et al., 1988, or i) which displays at least 60%, such as at least 70%, e.g. at least 75%, or at least 80%, e.g. at least 85%, at least 90% or at least 95% homology
- 20 with at least one of said amino acid sequences and/or ii) displays immunological cross-reactivity with an antibody raised against at least one of said α -amylases, and/or iii) is encoded by a DNA sequence which hybridizes to the DNA sequences encoding the above specified α -amylases which are apparent from
- 25 SEQ ID Nos. 1, 3 and 5 of the present application, and SEQ ID NO 4 and 5 of WO 95/26397, respectively.

- In connection with property i) the "homology" may be determined by use of any conventional algorithm, preferably by use of the
- 30 GAP programme from the GCG package version 7.3 (June 1993) using default values for GAP penalties (Genetic Computer Group (1991) Programme Manual for the GCG Package, version 7, 575 Science Drive, Madison, Wisconsin, USA 53711).

- 35 Property ii) of the α -amylase, i.e. the immunological cross reactivity, may be assayed using an antibody raised against or reactive with at least one epitope of the relevant Termamyl-like α -amylase. The antibody, which may either be monoclonal or

- polyclonal, may be produced by methods known in the art, e.g. as described by Hudson et al., 1989. The immunological cross-reactivity may be determined using assays known in the art, examples of which are Western Blotting or radial immunodiffusion assay, e.g. as described by Hudson et al., 1989. In this respect, immunological cross-reactivity between the α -amylases having the amino acid sequences SEQ ID Nos. 2, 4 and 6, respectively, has been found.
- 10 The oligonucleotide probe used in the characterization of the Termamyl-like α -amylase in accordance with property iii) above may suitably be prepared on the basis of the full or partial nucleotide or amino acid sequence of the α -amylase in question. Suitable conditions for testing hybridization involve
- 15 presoaking in 5xSSC and prehybridizing for 1h at -40°C in a solution of 20% formamide, 5xDenhardt's solution, 50mM sodium phosphate, pH 6.8, and 50 μg of denatured sonicated calf thymus DNA, followed by hybridization in the same solution supplemented with 100 μM ATP for 18h at -40°C , or other methods
- 20 described by e.g. Sambrook et al., 1989.

In the present context, "derived from" is intended not only to indicate an α -amylase produced or producible by a strain of the organism in question, but also an α -amylase encoded by a DNA

25 sequence isolated from such strain and produced in a host organism transformed with said DNA sequence. Finally, the term is intended to indicate an α -amylase which is encoded by a DNA sequence of synthetic and/or cDNA origin and which has the identifying characteristics of the α -amylase in question. The

30 term is also intended to indicate that the parent α -amylase may be a variant of a naturally occurring α -amylase, i.e. a variant which is the result of a modification (insertion, substitution, deletion) of one or more amino acid residues of the naturally occurring α -amylase.

Parent hybrid α -amylases

The parent α -amylase (being a Termamyl-like or non-Termamyl-like α -amylase) may be a hybrid α -amylase, i.e. an α -amylase
5 which comprises a combination of partial amino acid sequences derived from at least two α -amylases.

The parent hybrid α -amylase may be one which on the basis of amino acid homology and/or immunological cross-reactivity
10 and/or DNA hybridization (as defined above) can be determined to belong to the Termamyl-like α -amylase family. In this case, the hybrid α -amylase is typically composed of at least one part of a Termamyl-like α -amylase and part(s) of one or more other α -amylases selected from Termamyl-like α -amylases or non-
15 Termamyl-like α -amylases of microbial (bacterial or fungal) and/or mammalian origin.

Thus, the parent hybrid α -amylase may comprise a combination of at least two Termamyl-like α -amylases, or of at least one
20 Termamyl-like and at least one non-Termamyl-like bacterial α -amylase, or of at least one Termamyl-like and at least one fungal α -amylase. For instance, the parent α -amylase comprises a C-terminal part of an α -amylase derived from a strain of *B. licheniformis* and a N-terminal part of an α -amylase derived
25 from a strain of *B. amyloliquefaciens* or from a strain of *B. stearothermophilus*. For instance, the parent α -amylase comprises at least 430 amino acid residues of the C-terminal part of the *B. licheniformis* α -amylase, and may, e.g. comprise
a) an amino acid segment corresponding to the 37 N-terminal
30 amino acid residues of the *B. amyloliquefaciens* α -amylase having the amino acid sequence shown in SEQ ID No. 4 and an amino acid segment corresponding to the 445 C-terminal amino acid residues of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2, or b) an amino acid
35 segment corresponding to the 68 N-terminal amino acid residues of the *B. stearothermophilus* α -amylase having the amino acid sequence shown in SEQ ID No. 6 and an amino acid segment corresponding to the 415 C-terminal amino acid residues of the

B. licheniformis α -amylase having the amino acid sequence shown in SEQ ID No. 2.

Analogously, the parent hybrid α -amylase may belong to a non-
5 Termamyl-like α -amylase family, e.g. the Fungamyl-like α -amylase family. In that case the hybrid may comprise at least one part of an α -amylase belonging to the non-Termamyl-like α -amylase family in combination with one or more parts derived from other α -amylases.

10

The three-dimensional Termamyl-like α -amylase structure

The Termamyl-like α -amylase which was used to elucidate the three-dimensional structure forming the basis for the present
15 invention consists of the 300 N-terminal amino acids of the *B. amyloliquefaciens* α -amylase (with the amino acid sequence shown in SEQ ID No. 4) and amino acids 301-483 of the C-terminal end of the *B. licheniformis* α -amylase with the amino acid sequence SEQ ID No. 2. The bacterial α -amylase belongs to the "Termamyl-
20 like α -amylase family" and the present structure is believed to be representative for the structure of any Termamyl-like α -amylase.

The structure of the α -amylase was solved in accordance with
25 the principle for X-ray crystallographic methods given in "X-Ray Structure Determination", Stout, G.K. and Jensen, L.H., John Wiley & Sons, inc. NY, 1989. The structural coordinates for the solved crystal structure of the α -amylase at 2.2 Å resolution using the isomorphous replacement method are given
30 in a standard PDB format (Brookhaven Protein Data Base) in Appendix 1. It is to be understood that Appendix 1 forms part of the present application.

Amino acid residues of the enzyme are identified by three-
35 letter amino acid code (capitalized letters).

The α -amylase structure is made up of three globular domains ordered A, B, and C with respect to sequence, which lie

approximately along a line in the order B, A, C. The domains can be defined as being residues 1-103 and 206-395 for domain A, residues 104-205 for domain B, and residues 396-483 for domain C, the numbers referring to the *B. licheniformis* α -amylase. This gives rise to an elongated molecule, the longest axis being about 85Å. The widest point perpendicular to this axis is approximately 50Å and spans the central A domain. The active site residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) are D323, D231 and E261.

10

Domain A

Domain A is the largest domain and contains the active site (comprised of a cluster of three amino acid residues placed at the bottom of a deep cleft in the enzyme's surface). Domain A of all known α -amylase structures have the same overall fold, viz. the (beta/alpha)₈ barrel with 8 central beta strands (number 1-8) and 8 flanking α -helices. The β -barrel is defined by McGregor op. cit. The C-terminal end of Beta strand 1 is connected to helix 1 by a loop denoted loop 1 and an identical pattern is found for the other loops. These loops show some variation in size and some can be quite extensive.

The 8 central Beta-strands in the (beta/alpha)₈ barrel superimpose well between the various known α -amylase structures, and this part of the structure, including the close surroundings of the active site located at the c-terminal end of the beta-strands, show high similarity between the different amylases.

30

The loops connecting beta-strands and alpha helices display high variations between alpha amylases. These loops constitute the structural context of the active site and the majority of the contacts to the substrate is found among residues located in these loops. Such important characteristics as substrate specificity, substrate binding, pH/activity profile, starch cleavage pattern are determined by the amino acids and the positions of same in these loops.

The substantial differences between the Fungamyl-like α -amylase structure and the structure of the Termamyl-like α -amylase disclosed herein which are found in loops 1, 2, 3, and 8 are visualized in the Figures.

5

Domain B

The Termamyl-like α -amylase structure has been found to comprise a special domain structure in the A domain's loop3, also called domain B. The structure of the Termamyl-like α -amylase B domain has never been seen before in any of the known α -amylase or (β / α)8-barrel proteins.

The domain B structure is a very compact domain having a very high number of charged residues. The B domain arises as an extension of the loop between strand 3 and helix 3 of domain A (shown in Fig. 7) and contains a 5 stranded antiparallel β -sheet structure containing at least one long loop structure and having the connectivity -1, +3, -1X, +2 (Richardson, 1981, Adv. Protein Chem. 34, 167-339).

The first four strands of the B domain form two hairpin loops which twist around each other like a pair of crossed fingers (right-hand twist). The mainchain folds into a β -strand which connects two small β -sheet structures. After making one turn in one sheet it folds back and makes up a two stranded sheet in contact with domain A and an internal hole in the α -amylase structure. Then the mainchain folds up to a small sheet structure nearly perpendicular to the first two sheets. Before entering the helix 3 on top of the β -strand 3, the approximately 24 last amino acids in domain B form two calcium binding sites in the contact region to domain A.

Domain B is connected with domain A by two peptide stretches, which divide the domain-domain contact areas into two. Domain B is in contact with Domain A by a calcium binding region and an internally buried hole containing waters. Many types of molecular contacts are present. Ionic interacting between acid

and basic amino acids are possible, these interactions are very important for the general stability at high pH and for keeping the Calcium binding sites intact.

5 *Domain C*

Domain C is the C-terminal part of the protein consisting of amino acids 394-483. Domain C is composed entirely of β -strands which forms a single 8-stranded sheet structure, which folds
10 back on itself, and thus may be described as a β -sandwich structure. The connectivity is +1,+1, +5, -3, +1, +1, -3 although strands 6 and 7 are only loosely connected. One part of the β -sheet forms the interface to domain A.

15 *Ca-binding and Na-binding sites*

The structure of the Termamyl-like α -amylase is remarkable in that it exhibits four calcium-binding sites and one sodium-binding site. In other words four calcium ions and one sodium
20 ion are found to be present in the structure, although one of the calcium ions displays very weak coordination. Two of the calcium ions form part of a linear cluster of three ions, the central ion being attributed to sodium, which lie at the junction of the A and B domains.

25

The coordinating residues for the calcium ions between the A and B domain are as follows (using the Pdb file nomenclature for amino acid residues and atoms in the Pdb file found in Appendix 1 herein): For the calcium ion nearest to the active
30 site (IUM 502 in the pdb file), the backbone carbonyls from His235 and Asp194, the sidechain atom OD1 from residues Asp194, Asn102 and Asp200, and one water molecule WAT X3 (atom OW7). For the sodium ion (IUM 505), the binding site includes atom OD2 from Asp194, Asp200, Asp183 and Asp159, and a backbone
35 carbonyl from Val201. The coordinates for the other calcium ion between domain A and B are (IUM 501) : atom OD2 from Asp204 and Asp159, backbone carbonyl from Asp183 and Ala181, atom OD1 from Asp202, and one water molecule WAT X7 (atom OW7).

One calcium ion is located between the A and C domain, another is located in the C domain. The first mentioned calcium ion, which is also the one best coordinated (IUM 503) includes a carbonyl backbone from Gly300, Tyr302 and His406, atom OD2/OD1
5 from Asp430, atom OD1 from Asp407, and one water molecule WAT X6 (atom OW7). The other and very weakly coordinated calcium site (IUM 504) comprises 4 water molecules WAT X21 (atom OW8), X6 (atom OW6), X9 (atom OW0) and X28 (atom OW8), OE1/OE2 from Glu447 and OD1 from Asn444.

10

Substrate-binding site

Without being limited to any theory it is presently believed that favourable interactions between a substrate molecule and
15 the enzyme (such as hydrogen bonds and/or strong electrostatic interaction) are found within a sphere of 4Å of the substrate, when bound to the enzyme. The following residues of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2 are contemplated to be within a distance of 4 Å of
20 the substrate and thus believed to be involved in interactions with the substrate:

Trp13, Tyr14, Asn17, Asp18, Ser50, Gln51, Ala52, Asp53, Val54, Gly55, Tyr56, Lys70, Arg74, Lys76, Val102, His105, Gly107, Gly108, Ala109, Trp138, Thr163, Asp164, Trp165, Asn172, Glu189,
25 Tyr193, Leu196, Met197, Tyr198, Ala199, Arg229, Asp231, Ala232, Lys234, His235, Glu261, Trp263, His327, Asp328, Gln333, Ser334, and Leu335.

The amino acid residues of another Termamyl-like α -amylase,
30 which are contemplated to be within a distance of 4Å of the substrate, may easily be identified by aligning the amino acid sequence SEQ ID NO 2 with that of the other Termamyl-like α -amylase and thereby identifying the positions equivalent to those identified above.

35

Generality of structure

Because of the high homology between the various Termamyl-like α -amylases, the solved structure defined by the coordinates of Appendix 1 is believed to be representative for the structure of all Termamyl-like α -amylases. A model structure of other Termamyl-like α -amylases may easily be built on the basis of the coordinates given in Appendix 1 adapted to the α -amylase in question by use of an alignment between the respective amino acid sequences. The creation of a model structure is exemplified in Example 1.

The above identified structurally characteristic parts of the Termamyl-like α -amylase structure (Ca-binding site, substrate binding site, loops, etc.) may easily be identified in other Termamyl-like α -amylases on the basis of a model (or solved) structure of the relevant Termamyl-like α -amylase or simply on the basis of an alignment between the amino acid sequence of the Termamyl-like α -amylase in question with that of the *B. licheniformis* α -amylase used herein for identifying the amino acid residues of the respective structural elements.

Furthermore, in connection with Termamyl-like variants of the invention, which are defined by modification of specific amino acid residues of a specific Termamyl-like α -amylase, it will be understood that variants of another Termamyl-like α -amylase modified in an equivalent position (as determined from the best possible amino acid sequence alignment between the respective sequences) are intended to be covered as well. Thus, irrespective of whether an amino acid residue is identified herein for the purpose of defining a structural part of a given α -amylase or used for identifying a variant of the α -amylase, this amino acid residue shall be considered as representing the equivalent amino acid residue of any other Termamyl-like α -amylase.

Methods of the invention for design of novel α -amylase variants

In the methods according to the first, second and third aspects of the invention the terms "structure of a Termamyl-like α -amylase" and "Termamyl-like α -amylase structure" are intended to indicate the solved structure defined by the coordinates presented in Appendix 1 or a model structure of a given Termamyl-like α -amylase (such as the *B. licheniformis* α -amylase) built on the basis of the solved structure.

10

In most cases the parent Termamyl-like α -amylase to be modified in accordance with the present invention is different from the α -amylase which was actually used for solving the structure (Appendix 1). This means that the amino acid residue(s) or structural part(s) identified in the solved structure (Appendix 1) in step i) of the method according to the first, second or third aspect of the invention must be translated into the corresponding amino acid residue(s) or structural part(s) of the parent Termamyl-like α -amylase in question. The "translation" is conveniently performed on the basis of an amino acid sequence alignment between the amino acid sequence of the Termamyl-like α -amylase used for solving the structure and the amino acid sequence of the parent Termamyl-like α -amylase in question.

25

The analysis or comparison performed in step i) of the method according to the first, second and third aspect, respectively, of the invention may be performed by use of any suitable computer programme capable of analysing and/or comparing protein structures, e.g. the computer programme Insight, available from Biosym Technologies, Inc. For instance, the basic principle of structure comparison is that the three-dimensional structures to be compared are superimposed on the basis of an alignment of secondary structure elements (such as the central 8 β -strands in the barrel) and the parts differing between the structures can subsequently easily be identified from the superimposed structure.

The structural part which is identified in step i) of the methods of the first, second and third aspects of the invention may be composed of one amino acid residue. However, normally the structural part comprises more than one amino acid residue, typically constituting one of the above parts of the Termamyl-like α -amylase structure such as one of the A, B, or C domains, an interface between any of these domains, a calcium binding site, a loop structure, the substrate binding site, or the like.

10

In the present context the term "structural or functional considerations" is intended to indicate that modifications are made on the basis of an analysis of the relevant structure or structural part and its contemplated impact on the function of the enzyme. Thus, an analysis of the structures of the various α -amylases, which until now has been elucidated, optionally in combination with an analysis of the functional differences between these α -amylases, may be used for assigning certain properties of the α -amylases to certain parts of the α -amylase structure or to contemplate such relationship. For instance, differences in the pattern or structure of loops surrounding the active site may result in differences in access to the active site of the substrate and thus differences in substrate specificity and/or cleavage pattern. Furthermore, parts of a Termamyl-like α -amylase involved in or contemplated to be involved in substrate binding (and thus e.g. specificity/cleavage pattern), calcium or sodium ion binding (e.g. of importance for the Calcium-dependency of the enzyme), and the like has been identified (*vide infra*).

30

The modification of an amino acid residue or structural part is typically accomplished by suitable modifications of a DNA sequence encoding the parent enzyme in question. The term "modified" as used in step ii) in the method according to the first aspect of the invention is intended to have the following meaning: When used in relation to an amino acid residue the term is intended to mean replacement of the amino acid residue in question with another amino acid residue. When used in

relation to a structural part, the term is intended to mean replacement of one or more amino acid residues of said structural part, addition of one or more amino acid residues to said part, or deletion of one or more amino acid residues of
5 said structural part.

The construction of the variant of interest is accomplished by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing
10 the variant, and optionally subsequently recovering the variant from the resulting culture broth. This is described in detail further below.

First aspect of the invention

15 In a preferred embodiment of the method according to the first aspect of the invention the property of the parent enzyme to be modified is selected from calcium dependency, substrate binding, cleavage pattern, pH dependent activity and the like. Specific examples of how to change these properties of a parent
20 Termamyl-like α -amylase are given further below.

In another preferred embodiment the parent Termamyl-like α -amylase to be modified is a *B. licheniformis* α -amylase.

25 *Second and third aspects of the invention*

One important advantage of the methods according to the second and third aspects of the present invention is that it is possible to adapt the structure (or a structural part) of a Termamyl-like α -amylase to the structure (or structural part)
30 of a non-Termamyl-like α -amylase and *vide versa*. For instance, having identified a loop structure of the non-Termamyl-like α -amylase which is believed to be responsible for or contributing to a particular property of the non-Termamyl-like α -amylase it is possible to replace the corresponding structure of the
35 Termamyl-like α -amylase with said non-Termamyl-like α -amylase structure - or if no corresponding structure exists in the Termamyl-like α -amylase - to insert the structure into the Termamyl-like α -amylase in such a manner that the resulting

variant Termamyl-like α -amylase, as far as the relevant part is concerned, resembles the corresponding part of the non-Termamyl-like α -amylase. When two or more parts of the structure of the parent Termamyl-like α -amylase are modified so
5 as to resemble the corresponding parts of the non-Termamyl-like α -amylase it is possible to increase the resemblance to the non-Termamyl-like α -amylase of the Termamyl-like α -amylase variant and thus to alter the properties of said variant in the direction of those of said non-Termamyl-like α -amylase. Loop
10 modifications are discussed in much further detail further below.

Typically, the modification to be performed in step iii) of the method according to the second aspect of the invention is
15 accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified so as to adapt the structure of said part of the parent α -amylase to the corresponding part of the non-Termamyl-like α -amylase; by replacing one or more amino acid residues of the part of the
20 Termamyl-like α -amylase to be modified with the amino acid residues occupying corresponding positions in the non-Termamyl-like α -amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α -amylase into a corresponding position in the Termamyl-like α -amylase. For the
25 method according to the third aspect the modification is to be understood analogously, performed on the non-Termamyl-like parent α -amylase rather than the Termamyl-like α -amylase.

In step ii) of the method according to the second or third
30 aspect of the invention the part of the structure to be identified is preferably one which in the folded enzyme is believed to be in contact with the substrate (cf the disclosure above in the section entitled "Substrate-binding site) or involved in substrate specificity and/or cleavage pattern,
35 and/or one which is in contact with one of the calcium or sodium ions and/or one, which is contributing to the pH or temperature profile of the enzyme, or one which otherwise, from structural or functional considerations, is contemplated to be

responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α -amylase.

Non-Termamyl-like α -amylase

5 The non-Termamyl-like α -amylase with which the comparison is made in step i) of the method of the second aspect of the invention and which is the parent α -amylase in the method of the third aspect of the invention, may be any α -amylase, which does not belong to the family of Termamyl-like α -amylases (as
10 defined above) and, which as a consequence thereof, has a different three-dimensional structure. Furthermore, the non-Termamyl-like α -amylase should be one which has, at the time that the method is performed, an elucidated or contemplated three-dimensional structure.

15

The non-Termamyl-like α -amylase may, e.g., be a fungal α -amylase, a mammalian or a plant α -amylase or a bacterial α -amylase (different from a Termamyl-like α -amylase). Specific examples of such α -amylases include the *Aspergillus oryzae* TAKA
20 α -amylase, the *A. niger* acid α -amylase, the *Bacillus subtilis* α -amylase, the porcine pancreatic α -amylase and a barley α -amylase. All of these α -amylases have elucidated structures which are clearly different from the structure of the Termamyl-like α -amylase shown herein.

25

The fungal α -amylases mentioned above, i.e. derived from *A. niger* and *A. oryzae*, are highly homologous on the amino acid level and generally considered to belong to the same family of α -amylases. In the present disclosure, this family is termed
30 "Fungamyl-like α -amylase" and intends to indicate an α -amylase which exhibits a high homology, i.e. more than 70%, such as 80% homologous (as defined herein) to the fungal α -amylase derived from *Aspergillus oryzae*, commercially available as Fungamyl[®], and the *A. niger* α -amylase.

35

From the enclosed illustrations of the α -amylase structure of a Termamyl-like α -amylase and a comparison of said structure with the structure of a Fungamyl-like α -amylase it is evident

that major differences exist between the two structures. In the method of the invention it is of particular interest to modify parts of the parent Termamyl-like α -amylase, which belong to a region with large differences to the Fungamyl-like α -amylase. In particular, it is of interest to modify the parent Termamyl-like α -amylase in one or more of the following loops: loop 1, loop 2, loop 3 and/or loop 8 of the parent α -amylase.

In the method of the third aspect of the invention it is of particular interest to modify loop 1, loop 2, loop 3 and/or loop 8 of the parent non-Termamyl-like α -amylase to a closer resemblance to the similar loops of a Termamyl-like α -amylase, such as Termamyl.

In the following specific types of variants are described which have been designed by use of the method of the invention.

Loop modifications

In order to change the substrate specificity of the parent α -amylase to be modified it is relevant to consider loop modifications. For instance changing one or more of the loop structures of the Termamyl-like α -amylase into a closer resemblance with the corresponding loop structure(s) of a non-Termamyl-like α -amylase (such as a Fungamyl-like α -amylase) it is contemplated that it is possible to change the substrate specificity in the direction of that of the non-Termamyl α -amylase. In the following different types of loop modifications of interest are listed. It will be understood that the variants may have other changed properties in addition to the modified substrate specificity. It will be understood that the following modifications identified for a specific Termamyl-like α -amylase are intended to include corresponding modifications in other equivalent positions of other Termamyl-like α -amylases. Furthermore, it will be understood that, normally, the loop modification will comprise replacement of an entire loop structure or a substantial part thereof in, e.g., the Termamyl-

like α -amylase, with the corresponding loop structure (or substantial part thereof) in a non-Termamyl-like α -amylase.

Loop2 modifications

5 In one embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one amino acid residue of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ ID No. 4, i.e. loop 2,
10 has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No.
15 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

The amino acid sequence shown in SEQ ID No. 10 is the amino acid sequence of the *A. oryzae* α -amylase, i.e. a Fungamyl-like
20 α -amylase. It will be understood that amino acid residues or fragments found in corresponding positions in other α -amylases, in particular Fungamyl-like α -amylases, may be used as a template for the construction of the variant according to the invention. The corresponding part in other homologous α -
25 amylases may easily be identified on the basis of a comparison of the amino acid sequences and/or three-dimensional structures of the respective α -amylases.

For instance, the variant may be one, which, when the amino
30 acid sequence of the variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% such as at least 90% sequence homology with the part of SEQ ID No 10 extending
35 from residue Z to residue V of SEQ ID No 10, wherein X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,
Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and
5 V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

In other words, the variant may be one in which an amino acid fragment X-Y of the parent α -amylase, which corresponds to or
10 is within the amino acid fragment 44-57 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, in X, Y, Z and V have the meaning indicated above.

15

A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α -amylase, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 48-51 of SEQ ID No. 4, has been replaced
20 with an amino acid fragment corresponding to amino acid residues 70-78 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - limited alteration

25 In another embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 195-202 of the amino acid sequence of SEQ
30 ID No. 4, has been deleted or replaced with one or more of the amino acid residues which is/are present in an amino acid fragment corresponding to the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the
35 relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one in which an amino acid fragment X-Y of the parent α -amylase which corresponds to or is within the amino acid fragment 195-202 of SEQ ID No. 4, has been replaced by an amino acid fragment Z-V, which corresponds
5 to or is within the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, in which

X is an amino acid residue corresponding to the amino acid occupying position 195 or 196 of SEQ ID No. 4,

10

Y is an amino acid residue corresponding to the amino acid occupying position 198, 199, 200, 201, or 202 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid
15 occupying position 165 or 166 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 173, 174, 175, 176 or 177 of SEQ ID No. 10.

20 Expressed in another manner, the variant according to this aspect may be one, which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent Termamyl-like α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID
25 No 4, the said region having at least 80%, such as 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, the meaning of X, Y, Z and V being as identified above.

30 A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α -amylase, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino
35 acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - complete domain B

In a further embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which
5 is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino
10 acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

15 For instance, the variant may be one, in which an amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-210 of
20 the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,
25

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,
Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and
30

V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

A specific example of a variant according to this embodiment is
35 a variant of a parent α -amylase, in which an amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with

the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

In another embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-177 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-202 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

30

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

A specific example of a variant according to this embodiment of the invention is a variant, in which the amino acid fragment of

the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

5

Loop 1 modifications - minimal addition

In a further embodiment the present invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -
10 amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to
15 the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

20 For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 12-19 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 28-42 of
25 the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

30

Y is an amino acid residue corresponding to the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid
35 occupying position 28, 29, 30, 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

A specific example of a variant according to this aspect of the invention is a variant, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid
5 fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

Loop 1 modifications - complete loop

In a further embodiment the invention relates to a variant of
10 a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which
15 is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as
20 a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 7-23 of SEQ ID No. 4,
25 has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 13-45 of the amino acid sequence shown in SEQ ID No. 10, in which variant

30 X is an amino acid residue corresponding to the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,
35

Z is an amino acid residue corresponding to the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

A specific variant according to this embodiment is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

10

Loop 8 modifications

In a further embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 322-346 of SEQ ID No. 2, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 291-313 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

35

Y is an amino acid residue corresponding to the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is an amino acid residue corresponding to the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

A specific variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

Ca²⁺ dependency

It is highly desirable to be able to decrease the Ca²⁺ dependency of a Termamyl-like α -amylase. Accordingly, in a further aspect the invention relates to a variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a decreased Ca²⁺ dependency as compared to the parent α -amylase. The decreased Ca²⁺ dependency has the functional result that the variant exhibits a satisfactory amylolytic activity in the presence of a lower concentration of calcium ion in the extraneous medium than is necessary for the parent enzyme and, for example, therefore is less sensitive than the parent to calcium ion-depleting conditions such as those obtained in media containing calcium-complexing agents (such as certain detergent builders).

The decreased Ca²⁺ dependency of the variant of the invention may advantageously be achieved by increasing the Ca²⁺ binding affinity of the parent Termamyl-like α -amylase, in other words the stronger the Ca²⁺ binding of the enzyme, the lower is the Ca²⁺ dependency.

It is presently believed that amino acid residues located within 10Å from a sodium or calcium ion are involved in or are of importance for the Ca²⁺ binding capability of the enzyme.

Accordingly, the variant according to this aspect of the invention is preferably one, which has been modified in one or more amino acid residues present within 10Å from a calcium and/or sodium ion identified in the three-dimensional Termamyl-like α -amylase structure in such a manner that the affinity of the α -amylase for calcium is increased.

The amino acid residues found within a distance of 10Å from the Ca^{2+} binding sites of the *B. licheniformis* α -amylase with the amino acid sequence SEQ ID NO 2 were determined as described in Example 2 and are as follows:

V102, I103, N104, H105, K106, R125, W155, W157, Y158, H159, F160, D161, G162, T163, Y175, K176, F177, G178, K180, A181, W182, D183, W184, E185, V186, S187, N192, Y193, D194, Y195, L196, M197, Y198, A199, D200, I201, D202, Y203, D204, H205, P206, V208, A209, D231, A232, V233, K234, H235, I236, K237, F238, F240, L241, A294, A295, S296, T297, Q298, G299, G300, G301, Y302, D303, M304, R305, K306, L307, W342, F343, L346, Q393, Y394, Y396, H405, H406, D407, I408, V409, R413, E414, G415, D416, S417, V419, A420, N421, S422, G423, L424, I428, T429, D430, G431, P432, V440, G441, R442, Q443, N444, A445, G446, E447, T448, W449, I462, G475, Y480, V481, Q482, R483.

In order to construct a variant according to this aspect of the invention it is desirable to replace at least one of the above mentioned amino acid residues (or an amino acid residue occupying an equivalent position in another Termamyl-like α -amylase than that defined by SEQ ID NO 2), which is contemplated to be involved in providing a non-optimal calcium binding, with any other amino acid residue which improves the Ca^{2+} binding affinity of the variant enzyme. In practice, the identification and subsequent modification of the amino acid residue is performed by the following method:

35

i) identifying an amino acid residue within 10Å from a Ca^{2+} binding site of a Termamyl-like α -amylase structure, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,

ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and testing the Ca^{2+} dependency of the resulting Termamyl-like α -amylase variant.

10 In the present context, the term "non-optimal calcium ion interaction" is intended to indicate that the amino acid residue in question is selected on the basis of a presumption that substituting said amino acid residue for another may improve a calcium ion binding interaction of the enzyme. For
15 instance, the amino acid residue in question may be selected on the basis of one or more of the following considerations:

- to obtain an improved interaction between a calcium ion and an amino acid residue located near to the surface of the enzyme
20 (as identified from the structure of the Termamyl-like α -amylase). For instance, if the amino acid residue in question is exposed to a surrounding solvent, it may be advantageous to increase the shielding of said amino acid residue from the solvent so as to provide for a stronger interaction between
25 said amino acid residue and a calcium ion. This can be achieved by replacing said residue (or an amino acid residue in the vicinity of said residue contributing to the shielding) by an amino acid residue which is more bulky or otherwise results in an improved shielding effect.

30

- to stabilize a calcium binding site, for instance by stabilizing the structure of the Termamyl-like α -amylase (e.g. by stabilizing the contacts between the A, B and C domains or stabilizing one or more of the domains as such). This may,
35 e.g., be achieved by providing for a better coordination to amino acid side chains, which may, e.g., be obtained by replacing an N residue with a D residue and/or a Q residue with

an E residue (e.g. N104D), e.g. within 10Å, and preferably within 3 or 4Å, of a calcium binding site.

- to protect the calcium binding site or to improve the coordination between the calcium ion and the calcium binding site, e.g. by providing a stronger interaction between the ion and the binding site.

Before actually constructing a Termamyl-like α -amylase variant according to the above principles it may be convenient to evaluate the contemplated amino acid modification by its accommodation into the Termamyl-like α -amylase structure, e.g. into a model structure of the parent Termamyl-like α -amylase.

Preferably, the amino acid residue to be modified is located within 8Å of a Ca^{2+} binding site residue, such as within 5Å of such residue. The amino acid residues within 8Å and 5Å, respectively, may easily be identified by an analogous method used for identifying amino acid residues within 10Å (cf. Example 2).

The following mutation is contemplated to be of particular interest with respect to decreasing the Ca^{2+} dependency of a Termamyl-like α -amylase:

N104D (of the *B. licheniformis* α -amylase SEQ ID NO 2, or an equivalent (N to D) mutation of an equivalent position in another Termamyl-like α -amylase.)

In connection with substitutions of relevance for Ca^{2+} dependency, some other substitutions appear to be of importance in stabilizing the enzyme conformation (for instance the Domains A-B and/or Domains A-C interactions contributing to the overall stability of the enzyme) in that they may, e.g., enhance the strength of binding or retention of calcium ion or sodium ion at or within a calcium or sodium binding site, respectively, within the parent Termamyl-like α -amylase.

It is desirable to stabilize the C-domain in order to increase the calcium stability and/or thermostability of the enzyme. In this connection the stabilization may result in a stabilization of the binding of calcium by the enzyme, and an improved contact between the C-domain and the A-domain (of importance for thermostability). The latter may be achieved by introduction of cystein bridges, salt bridges or increase hydrogen, hydrophobic and/or electrostatic interactions.

For instance, the C-domain of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2 may be stabilized by introduction of a cystein bridge between domain A and domain C, e.g. by introducing of the following mutations: A349C+I479C and/or L346C+I430C.

15

A salt bridge may be obtained by introduction of the following mutations:

N457D,E

N457D,E+K385R

20 F350D,E+I430R,K

F350D,E+I411R,K

The calcium site of Domain C may be stabilized by replacing the amino acid residues H408 and/or G303 with any other amino acid residue. Of particular interest is the following mutations:

H408Q,E,N,D and/or G303N,D,Q,E

which are contemplated to provide a better calcium binding or protection from calcium depletion.

Similar mutations may be introduced in equivalent positions of other Termamyl-like α -amylases.

Other substitution mutations (relative to *B. licheniformis* α -amylase, SEQ ID No. 2) which appear to be of importance, *inter alia*, in the context of reducing calcium dependency include the following: R23K, H156Y, A181T, A209V and G310D (or equivalent mutations in equivalent positions in another Termamyl-like α -amylase). Substitutions of R214 and P345 with

other amino acids may also be of importancen in this connection.

Variants with altered activity at higher/lower pH

5

It is contemplated that it is possible to change the pH optima of a Termamyl-like α -amylase or the enzymatic activity at a given pH by changing the pKa of the active site residues. This may be achieved, e.g. by changing the electrostatic interaction
10 or hydrophobic interaction between functional groups of amino acid side chains of the amino acid residue to be modified and of its close surroundings. This may, e.g., be accomplished by the following method:

15 i) in a structure of the Termamyl-like α -amylase in question to identifying an amino acid residue within 15Å from an active site residue, in particular 10Å from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site
20 residue,

ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and
25 evaluating the accomodation of the amino acid residue in the structure,

iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into
30 the structure,

iv) constructing a Termamyl-like α -amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent enzymatic activity of interest of said variant.

35

In the above method it may be of particular relevance to add a positively charged residue within 5Å of a glutamate (thereby lowering the pKa of the glutamate from about 4.5 to 4), or to

add a negatively charged residue within 5 Å of a glutamate (thereby increasing the pKa to about 5), or to make similar modifications within a distance of about 5Å of a Histidine.

5 In a further aspect the invention relates to a variant of a Termamyl-like α -amylase which exhibits a higher activity at a lower pH (e.g. compared to the pH optimum) than the parent α -amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the
10 following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

E336, Q333, P331, I236, V102, A232, I103, L196

The following mutations are of particular interest:

15

E336R, K

Q333R, K

P331R, K

V102R, K, A, T, S, G;

20 I236K, R, N;

I103K, R;

L196K, R;

A232T, S, G;

25 or any combination of two or more of these variants or any combination of one or more of these variants with any of the other variants disclosed herein.

In a still further aspect the invention relates to a variant of
30 a Termamyl-like α -amylase which has a higher activity at a higher pH than the parent α -amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

35

N236, H281, Y273

In particular, the variant comprises a mutation corresponding to at least one of the following mutations of the *B. licheniformis* α -amylase (SEQ ID NO 2):

5 N326I,Y,F,L,V
H281F,I,L
Y273F,W

or any combination of two or more of these variants or any
10 combination of one or more of these variants with any of
the other variants disclosed herein.

A mutation which appears to be importance in relation to the specific activity of variants of the invention is a mutation
15 corresponding to the substitution S187D in *B. licheniformis* α -amylase (SEQ ID NO 2).

Variants with increased thermostability and/or altered
temperature optimum

20

In a further desired aspect the invention relates to a variant of a parent Termamyl-like α -amylase, which variant is the result of one or more amino acid residues having been deleted from, replaced or added to the parent α -amylase so as to obtain
25 an increased thermostability of the variant.

The Termamyl-like α -amylase structure contains a number of unique internal holes, which may contain water, and a number of crevices. In order to increase the thermostability of the α -
30 amylase it may be desirable to reduce the number of holes and crevices (or reduce the size of the holes or crevices), e.g. by introducing one or more hydrophobic contacts, preferably achieved by introducing bulkier residues, in the vicinity or surroundings of the hole. For instance, the amino acid residues
35 to be modified are those which are involved in the formation of the hole.

Accordingly, in a further aspect the present invention relates to a method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α -amylase, which method comprises

5

- i) identifying an internal hole or a crevice of the parent Termamyl-like α -amylase in the three-dimensional structure of said α -amylase,
 - 10 ii) replacing, in the structure, one or more amino acid residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of
 - 15 the hole or crevice,
 - iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.
- 20 The structure used for identifying the hole or crevice of the parent Termamyl-like α -amylase may be the structure identified in Appendix 1 or a model structure of the parent Termamyl-like α -amylase built thereon.
- 25 It will be understood that the hole or crevice is identified by the amino acid residues surrounding the hole/crevice, and that modification of said amino acid residues are of importance for filling or reducing the size of the hole/crevice. The particular amino acid residues referred to below are those
- 30 which in crystal structure have been found to flank the hole/crevice in question.

In order to fill (completely or partly) a major hole located between domain A and B, mutation to any other amino acid

35 residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143,
R146

5

Of particular interest is a mutation to a more bulky amino acid residue than the amino acid residue of the parent enzyme.

Of particular interest is a variant of a Termamyl-like α -
10 amylase which comprises a mutation corresponding to the following mutations (using the numbering of *B. licheniformis* α -amylase (SEQ ID NO 2)):

L61W,V,F;
15 Y62W;
F67W;
K106R,F,W;
G145F,W
I212F,L,W,Y,R,K;
20 S151 replaced with any other amino acid residue and in particular with F,W,I or L;
R214W;
Y150R,K;
F143W; and/or
25 R146W.

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues
30 of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L241, I236.

35 Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

5 L241I,F,Y,W; and/or
I236L,F,W,Y

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid
10 residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L7, V259, F284

15 Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

20 L7F,I,W
V259F,I,L
F284W

25 In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

30 F350, F343

Of interest is a mutation to a more bulky amino acid residue.

35 Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:
F350W

F343W

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L427, V481

10

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

L427F,L,W

V481,F,I,L,W

20 Variants with an altered cleavage pattern

In the starch liquefaction process it is desirable to use an α -amylase which is capable of degrading the starch molecules into long branched oligo saccharides (like, e.g. the Fungamyl-like α -amylases) rather than shorter branched oligo saccharides (like conventional Termamyl-like α -amylases). The resulting very small branched oligosaccharides (panose precursors) cannot be hydrolyzed properly by pullulanases, which in the liquefaction process are used after the α -amylases and before the amyloglucosidases. Thus, in the presence of panose precursors the action of amylo-glucoamylase ends up with a high degree of the small branched limiting-dextrin, the trisaccharide panose. The presence of panose lowers the saccharification yield significantly and is thus undesirable.

35 Thus, one aim of the present invention is to change the degradation characteristics of a Termamyl-like α -amylase to that of a Fungamyl-like α -amylases without at the same time reducing the thermostability of the Termamyl-like α -amylase.

Accordingly, in a further aspect the invention relates to a variant of a Termamyl-like α -amylase which has a reduced ability to cleave a substrate close to the branching point.

5 The variant may suitably be constructed by a method which comprises

i) identifying the substrate binding area of the parent Termamyl-like α -amylase in a model of the three-dimensional
10 structure of said α -amylase, (e.g. within a sphere of 4Å from the substrate binding site (as defined in the section above entitled "Substrate Binding Site"),

ii) replacing, in the model, one or more amino acid residues of
15 the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of the parent α -amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more
20 amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and

25 iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

Of particular interest is a variant which cleaves an
30 amylopectin substrate, from the reducing end, more than one glucose unit from the branching point, preferably more than two or three glucose units from the branching point, i.e. at a further distance from the branching point than that obtained by use of a wild type *B. licheniformis* α -amylase.

35

Residues of particular interest in connection with this aspect of the invention correspond to the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2): V54, D53, Y56, Q333,

G57, and the variants according to this aspect preferably comprises a mutation in one or more of these residues.

In particular, the variant comprises at least one of the
5 following mutations, which are expected to prevent cleavage close to the branching point:

V54L, I, F, Y, W, R, K, H, E, Q

D53L, I, F, Y, W

10 Y56W

Q333W

G57all possible amino acid residues

A52amino acid residues larger than A, e.g. A52W, Y, L, F, I.

15 Variants of a fungal α -amylase

In a still further embodiment the invention relates to a variant of a parent Fungamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -
20 amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid
25 residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α -amylase as a template.

30

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 10, has/have been replaced with an amino acid fragment Z-V, which
35 corresponds to or is within the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 4, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 10,

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

10 V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

A specific example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the
15 parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

20 Another example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the
25 amino acid sequence shown in SEQ ID No. 4.

In a further embodiment the invention relates to a variant of a parent Fungamyl-like α -amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the
30 amino acid sequence shown in SEQ ID No. 10 has been deleted.

General mutations in variants of the invention

It may be preferred that the variant of the invention or
35 prepared in accordance with the method of the invention comprises one or more modifications in addition to those outlined above. Thus, it may be advantageous that one or more proline residues present in the part of the α -amylase variant

having been modified is/are replaced with a non-proline residue which may be any of the possible, naturally occurring non-proline residues, and which preferably is an alanine, glycine, serine, threonine, valine or leucine.

5

Analogously, it may be preferred that one or more cysteine residues present in the amino acid residues with which the parent α -amylase is modified are replaced with a non-cysteine residues such as serine, alanine, threonine, glycine, valine or
10 leucine.

Furthermore, the variant of the invention may either as the only modification or in combination with any of the above outlined modifications be modified so that one or more Asp
15 and/or Glu present in an amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively. Also of interest is the modification of one or more of the Lys residues present in the Termamyl-like α -amylase is replaced by an Arg present in an
20 amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively.

It will be understood that in accordance with the present
25 invention variants may be prepared which carry two or more of the above outlined modifications. For instance, variants may be prepared which comprises a modification in the loop 1 and loop 2 region, a modification in loop 2 and limited loop 3, a modification in loop 1, loop 2, loop 3 and loop 8, etc.

30

Furthermore, it may be advantageous to introduce point-mutations in any of the variants described herein.

Methods of preparing α -amylase variants

35 Several methods for introducing mutations into genes are known in the art. After a brief discussion of the cloning of α -amylase-encoding DNA sequences, methods for generating

mutations at specific sites within the α -amylase-encoding sequence will be discussed.

Cloning a DNA sequence encoding an α -amylase

- 5 The DNA sequence encoding a parent α -amylase may be isolated from any cell or microorganism producing the α -amylase in question, using various methods well known in the art. First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that pro-
- 10 duces the α -amylase to be studied. Then, if the amino acid sequence of the α -amylase is known, homologous, labelled oligonucleotide probes may be synthesized and used to identify α -amylase-encoding clones from a genomic library prepared from the organism in question. Alternatively, a labelled oligonu-
- 15 cleotide probe containing sequences homologous to a known α -amylase gene could be used as a probe to identify α -amylase-encoding clones, using hybridization and washing conditions of lower stringency.
- 20 Yet another method for identifying α -amylase-encoding clones would involve inserting fragments of genomic DNA into an expression vector, such as a plasmid, transforming α -amylase-negative bacteria with the resulting genomic DNA library, and then plating the transformed bacteria onto agar containing a
- 25 substrate for α -amylase, thereby allowing clones expressing the α -amylase to be identified.

Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g.

30 the phosphoroamidite method described by S.L. Beaucage and M.H. Caruthers (1981) or the method described by Matthes et al. (1984). In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned in appropriate vectors.

35

Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by ligating fragments of synthetic,

genomic or cDNA origin (as appropriate, the fragments corresponding to various parts of the entire DNA sequence), in accordance with standard techniques. The DNA sequence may also be prepared by polymerase chain reaction (PCR) using specific
5 primers, for instance as described in US 4,683,202 or R.K. Saiki et al. (1988).

Site-directed mutagenesis

Once an α -amylase-encoding DNA sequence has been isolated, and
10 desirable sites for mutation identified, mutations may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites; mutant nucleotides are inserted during oligonucleotide synthesis. In a specific method, a single-stranded
15 gap of DNA, bridging the α -amylase-encoding sequence, is created in a vector carrying the α -amylase gene. Then the synthetic nucleotide, bearing the desired mutation, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment)
20 and the construct is ligated using T4 ligase. A specific example of this method is described in Morinaga et al. (1984). US 4,760,025 discloses the introduction of oligonucleotides encoding multiple mutations by performing minor alterations of the cassette. However, an even greater variety of mutations can
25 be introduced at any one time by the Morinaga method, because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method of introducing mutations into α -amylase-encoding
30 DNA sequences is described in Nelson and Long (1989). It involves the 3-step generation of a PCR fragment containing the desired mutation introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment carrying the mutation
35 may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

Random mutagenesis

Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

5

For region-specific random mutagenesis with a view to improving the thermal stability of a parent Termamyl-like α -amylase, codon positions corresponding to the following amino acid residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) may
10 appropriately be targeted:

To improve the stability of the calcium site between Domain A and C

I428-A435

15 T297-L308

F403-V409

To improve the stability between domain A and B:

D180-D204

20 H156-T163

A232-F238

With a view to achieving improved binding of a substrate (i.e. improved binding of a carbohydrate species, such as amylose or
25 amylopectin) by a Termamyl-like α -amylase variant, modified (e.g. higher) substrate specificity and/or modified (e.g. higher) specificity with respect to cleavage (hydrolysis) of substrate, it appears that the following codon positions for the amino acid sequence shown in SEQ ID NO 2 (or equivalent
30 codon positions for another parent Termamyl-like α -amylase in the context of the invention) may particularly appropriately be targeted:

13-18

35 50-56

70-76

102-109

163-172

189-199

229-235

360-264

327-335

5

The random mutagenesis of a DNA sequence encoding a parent α -amylase to be performed in accordance with step a) of the above-described method of the invention may conveniently be performed by use of any method known in the art.

10

For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents.

The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues.

When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

35

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleo-

tide at the positions which are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the amylolytic enzyme by any published technique, using e.g. PCR, LCR or any DNA polymerase and ligase.

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent α -amylase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., Technique, Vol.1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., Molec. Gen. Genet., 133, 1974, pp. 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the amylolytic enzyme by e.g. transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may subsequently be transformed into the expression organism.

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent amylolytic enzyme. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenizing agent. The DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harboured in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence prior to the expression step (b) or the screening step (c) being performed. Such amplification may be performed in

accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

5

Subsequent to the incubation with or exposure to the mutagenizing agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this
10 purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: grampositive bacteria such as *Bacillus subtilis*,
15 *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gramnegative
20 bacteria such as *E.coli*.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

25

Localized random mutagenesis: the random mutagenesis may advantageously be localized to a part of the parent α -amylase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular
30 importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

35

The localized random mutagenesis is conveniently performed by use of PCR-generated mutagenesis techniques as described above or any other suitable technique known in the art.

Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g. by being inserted into a suitable vector, and said part may subsequently be subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

With respect to the screening step in the above-mentioned method of the invention, this may conveniently be performed by use of an aa filter assay based on the following principle:

10

A microorganism capable of expressing the mutated amylolytic enzyme of interest is incubated on a suitable medium and under suitable conditions for the enzyme to be secreted, the medium being provided with a double filter comprising a first protein-binding filter and on top of that a second filter exhibiting a low protein binding capability. The microorganism is located on the second filter. Subsequent to the incubation, the first filter comprising enzymes secreted from the microorganisms is separated from the second filter comprising the microorganisms.

20 The first filter is subjected to screening for the desired enzymatic activity and the corresponding microbial colonies present on the second filter are identified.

The filter used for binding the enzymatic activity may be any protein binding filter e.g. nylon or nitrocellulose. The top-filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins e.g. cellulose acetate or Durapore™. The filter may be pretreated with any of the conditions to be used for screening or may be treated during the detection of enzymatic activity.

The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any other known technique for detection of enzymatic activity.

35

The detecting compound may be immobilized by any immobilizing agent e.g. agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents.

α -Amylase activity is detected by Cibacron Red labelled amylopectin, which is immobilized on agarose. For screening for variants with increased thermal and high-pH stability, the filter with bound α -amylase variants is incubated in a buffer
5 at pH 10.5 and 60° or 65°C for a specified time, rinsed briefly in deionized water and placed on the amylopectin-agarose matrix for activity detection. Residual activity is seen as lysis of Cibacron Red by amylopectin degradation. The conditions are chosen to be such that activity due to the α -amylase having the
10 amino acid sequence shown in SEQ ID No.1 can barely be detected. Stabilized variants show, under the same conditions, increased colour intensity due to increased liberation of Cibacron Red.

15 For screening for variants with an activity optimum at a lower temperature and/or over a broader temperature range, the filter with bound variants is placed directly on the amylopectin-Cibacron Red substrate plate and incubated at the desired temperature (e.g. 4°C, 10°C or 30°C) for a specified time.
20 After this time activity due to the α -amylase having the amino acid sequence shown in SEQ ID No.1 can barely be detected, whereas variants with optimum activity at a lower temperature will show increase amylopectin lysis. Prior to incubation onto the amylopectin matrix, incubation in all kinds of desired
25 media - e.g. solutions containing Ca²⁺, detergents, EDTA or other relevant additives - can be carried out in order to screen for changed dependency or for reaction of the variants in question with such additives.

30

Testing of variants of the invention

The testing of variants of the invention may suitably be performed by determining the starch-degrading activity of the
35 variant, for instance by growing host cells transformed with a DNA sequence encoding a variant on a starch-containing agarose plate and identifying starch-degrading host cells. Further testing as to altered properties (including specific activity,

substrate specificity, cleavage pattern, thermoactivation, pH optimum, pH dependency, temperature optimum, and any other parameter) may be performed in accordance with methods known in the art.

5

Expression of α -amylase variants

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in enzyme form,
10 using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

15 The recombinant expression vector carrying the DNA sequence encoding an α -amylase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector will often depend on the host cell into which it is to be introduced. Thus, the vector
20 may be an autonomously replicating vector, i.e. a vector which exists as an extrachromosomal entity, the replication of which is independent of chromosomal replication, e.g. a plasmid, a bacteriophage or an extrachromosomal element, minichromosome or an artificial chromosome. Alternatively, the vector may be one
25 which, when introduced into a host cell, is integrated into the host cell genome and replicated together with the chromosome(s) into which it has been integrated.

In the vector, the DNA sequence should be operably connected to
30 a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell. Examples of suitable promoters for directing the transcription of the DNA
35 sequence encoding an α -amylase variant of the invention, especially in a bacterial host, are the promoter of the lac operon of *E.coli*, the *Streptomyces coelicolor* agarase gene *dagA* promoters, the promoters of the *Bacillus licheniformis* α -

amylase gene (*amyL*), the promoters of the *Bacillus*
stearothermophilus maltogenic amylase gene (*amyM*), the promo-
ters of the *Bacillus amyloliquefaciens* α -amylase (*amyQ*), the
promoters of the *Bacillus subtilis* *xylA* and *xylB* genes etc. For
5 transcription in a fungal host, examples of useful promoters
are those derived from the gene encoding *A. oryzae* TAKA
amylase, *Rhizomucor miehei* aspartic proteinase, *A. niger* neu-
tral α -amylase, *A. niger* acid stable α -amylase, *A. niger* glu-
coamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline
10 protease, *A. oryzae* triose phosphate isomerase or *A. nidulans*
acetamidase.

The expression vector of the invention may also comprise a
suitable transcription terminator and, in eukaryotes, poly-
15 adenylation sequences operably connected to the DNA sequence
encoding the α -amylase variant of the invention. Termination
and polyadenylation sequences may suitably be derived from the
same sources as the promoter.

20 The vector may further comprise a DNA sequence enabling the
vector to replicate in the host cell in question. Examples of
such sequences are the origins of replication of plasmids
pUC19, *pACYC177*, *pUB110*, *pE194*, *pAMB1* and *pIJ702*.

25 The vector may also comprise a selectable marker, e.g. a gene
the product of which complements a defect in the host cell,
such as the *dal* genes from *B. subtilis* or *B. licheniformis*, or
one which confers antibiotic resistance such as ampicillin,
kanamycin, chloramphenicol or tetracyclin resistance. Fur-
30 thermore, the vector may comprise *Aspergillus* selection markers
such as *amdS*, *argB*, *niaD* and *sC*, a marker giving rise to
hygromycin resistance, or the selection may be accomplished by
co-transformation, e.g. as described in WO 91/17243.

35 While intracellular expression may be advantageous in some
respects, e.g. when using certain bacteria as host cells, it is
generally preferred that the expression is extracellular. In
general, the *Bacillus* α -amylases mentioned herein comprise a

preregion permitting secretion of the expressed protease into the culture medium. If desirable, this preregion may be replaced by a different preregion or signal sequence, conveniently accomplished by substitution of the DNA sequences encoding the respective preregions.

The procedures used to ligate the DNA construct of the invention encoding an α -amylase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of an α -amylase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are grampositive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, or *Streptomyces lividans* or *Streptomyces*

murinus, or gramnegative bacteria such as *E.coli*. The transformation of the bacteria may, for instance, be effected by protoplast transformation or by using competent cells in a manner known *per se*.

5

The yeast organism may favourably be selected from a species of *Saccharomyces* or *Schizosaccharomyces*, e.g. *Saccharomyces cerevisiae*. The filamentous fungus may advantageously belong to a species of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergil-*
10 *lus niger*. Fungal cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells is described in EP 238 023.

15

In a yet further aspect, the present invention relates to a method of producing an α -amylase variant of the invention, which method comprises cultivating a host cell as described above under conditions conducive to the production of the
20 variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and
25 obtaining expression of the α -amylase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

30 The α -amylase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium
35 sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

Industrial Applications

The α -amylase variants of this invention possesses valuable properties allowing for various industrial applications. In particular the enzyme variants finds potential applications as
5 a component in washing, dishwashing and hard surface cleaning detergent compositions, but it may also be useful in the production of sweeteners and ethanol from starch and for textile desizing. Conditions for conventional starch converting processes and liquefaction and/or saccharification processes
10 are described in for instance US Patent No. 3,912,590 and EP patent publications Nos. 252,730 and 63,909.

Production of sweetners from starch: A "traditional" process for conversion of starch to fructose syrups normally consists
15 of three consecutive enzymatic processes, viz. a liquefaction process followed by a saccharification process and an isomerization process. During the liquefaction process, starch is degraded to dextrins by an α -amylase (e.g. Termamyl™) at pH values between 5.5 and 6.2 and at temperatures of 95-160°C for
20 a period of approx. 2h. In order to ensure an optimal enzyme stability under these conditions, 1mM of calcium is added (40 ppm free calcium ions).

After the liquefaction process the dextrins are converted into
25 dextrose by addition of a glucoamylase (e.g. AMG™) and a debranching enzyme, such as an isoamylase or a pullulanase (e.g. Promozyme™). Before this step the pH is reduced to a value below 4.5, maintaining the high temperature (above 95°C), and the liquefying α -amylase activity is denatured. The tem-
30 perature is lowered to 60°C, and glucoamylase and debranching enzyme are added. The saccharification process proceeds for 24-72 hours.

After the saccharification process the pH is increased to a
35 value in the range of 6-8, preferably pH 7.5, and the calcium is removed by ion exchange. The dextrose syrup is then converted into high fructose syrup using, e.g., an immobilized glucoseisomerase (such as Sweetzyme™).

At least 3 enzymatic improvements of this process could be obtained. All three improvements could be seen as individual benefits, but any combination (e.g. 1+2, 1+3, 2+3 or 1+2+3) could be employed:

5

Improvement 1. Reduction of the calcium dependency of the liquefying α -amylase.

Addition of free calcium is required to ensure adequately high
10 stability of the α -amylase, but free calcium strongly inhibits the activity of the glucose isomerase and needs to be removed, by means of an expensive unit operation, to an extent which reduces the level of free calcium to below 3-5 ppm. Cost savings could be obtained if such an operation could be avoided
15 and the liquefaction process could be performed without addition of free calcium ions.

To achieve that, a less calcium-dependent Termamyl-like α -amylase which is stable and highly active at low
20 concentrations of free calcium (< 40 ppm) is required. Such a Termamyl-like α -amylase should have a pH optimum at a pH in the range of 4.5-6.5, preferably in the range of 4.5-5.5.

Improvement 2. Reduction of formation of unwanted Maillard
25 products

The extent of formation of unwanted Maillard products during the liquefaction process is dependent on the pH. Low pH favours reduced formation of Maillard products. It would thus be
30 desirable to be able to lower the process pH from around pH 6.0 to a value around pH 4.5; unfortunately, all commonly known, thermostable Termamyl-like α -amylases are not very stable at low pH (i.e. pH < 6.0) and their specific activity is generally low.

35

Achievement of the above-mentioned goal requires a Termamyl-like α -amylase which is stable at low pH in the range of

4.5-5.5 and at free calcium concentrations in the range of 0-40 ppm, and which maintains a high specific activity.

Improvement 3.

5

It has been reported previously (US patent 5,234,823) that when saccharifying with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase, the presence of residual α -amylase activity from the liquefaction process can lead to lower yields of
10 dextrose if the α -amylase is not inactivated before the saccharification stage. This inactivation can typically be carried out by adjusting the pH to below 4.3 at 95°C, before lowering the temperature to 60°C for saccharification.

15 The reason for this negative effect on dextrose yield is not fully understood, but it is assumed that the liquefying α -amylase (for example Termamyl™ 120 L from *B. licheniformis*) generates "limit dextrins" (which are poor substrates for *B. acidopullulyticus* pullulanase) by hydrolysing 1,4-alpha-
20 glucosidic linkages close to and on both sides of the branching points in amylopectin. Hydrolysis of these limit dextrins by glucoamylase leads to a build-up of the trisaccharide panose, which is only slowly hydrolysed by glucoamylase.

25 The development of a thermostable α -amylase which does not suffer from this disadvantage would be a significant process improvement, as no separate inactivation step would be required.

30 If a Termamyl-like, low-pH-stable α -amylase is developed, an alteration of the specificity could be an advantage needed in combination with increased stability at low pH.

The methodology and principles of the present invention make it
35 possible to design and produce variants according to the invention having the required properties as outlined above.

Detergent Compositions

According to the invention, the α -amylase may typically be a component of a detergent composition. As such, it may be included in the detergent composition in the form of a non-dusting granulate, a stabilized liquid, or a protected enzyme.

5 Non-dusting granulates may be produced, e.g. as disclosed in US 4,106,991 and 4,661,452 (both to Novo Industri A/S) and may optionally be coated by methods known in the art. Examples of waxy coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to

10 20000, ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and mono- and di- and triglycerides of fatty acids. Examples of

15 film-forming coating materials suitable for application by fluid bed techniques are given in patent GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods.

20 Other enzyme stabilizers are well known in the art. Protected enzymes may be prepared according to the method disclosed in EP 238,216.

The detergent composition of the invention may be in any convenient form, e.g. as powder, granules, paste or liquid. A

25 liquid detergent may be aqueous, typically containing up to 70% of water and 0-30% of organic solvent, or nonaqueous.

The detergent composition comprises one or more surfactants, each of which may be anionic, nonionic, cationic, or zwitter-

30 ionic. The detergent will usually contain 0-50% of anionic surfactant such as linear alkylbenzenesulfonate (LAS), alpha-olefinsulfonate (AOS), alkyl sulfate (fatty alcohol sulfate) (AS), alcohol ethoxysulfate (AEOS or AES), secondary alkane-sulfonates (SAS), alpha-sulfo fatty acid methyl esters, alkyl-

35 or alkenylsuccinic acid or soap. It may also contain 0-40% of nonionic surfactant such as alcohol ethoxylate (AEO or AE), carboxylated alcohol ethoxylates, nonylphenol ethoxylate, alkylpolyglycoside, alkyltrimethylamineoxide, ethoxylated fatty

acid monoethanolamide, fatty acid monoethanolamide, or polyhydroxy alkyl fatty acid amide (e.g. as described in WO 92/06154).

- 5 The detergent composition may additionally comprise one or more other enzymes, such as lipase, cutinase, protease, cellulase, peroxidase, e.g., laccase.

The detergent may contain 1-65% of a detergent builder or
10 complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, citrate, nitrilotriacetic acid (NTA), ethylenediaminetetraacetic acid (EDTA), diethylenetriaminepentaacetic acid (DTMPA), alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst). The
15 detergent may also be unbuilt, i.e. essentially free of detergent builder.

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose (CMC), poly(vinylpyrrolidone) (PVP),
20 polyethyleneglycol (PEG), poly(vinyl alcohol) (PVA), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise
25 a H_2O_2 source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetylenediamine (TAED) or nonanoyloxybenzenesulfonate (NOBS). Alternatively, the bleaching system may comprise peroxy acids of e.g. the amide, imide, or sulfone
30 type.

The enzymes of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g. a polyol such as propylene glycol or glycerol, a sugar or sugar
35 alcohol, lactic acid, boric acid, or a boric acid derivative as e.g. an aromatic borate ester, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, or perfume.

The pH (measured in aqueous solution at use concentration) will usually be neutral or alkaline, e.g. 7-11.

10 Particular forms of detergent compositions within the scope of the invention include:

1) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

	Linear alkylbenzenesulfonate (calculated as acid)	7	-	12%
20	Alcohol ethoxysulfate (e.g. C ₁₂₋₁₈ alcohol, 1-2 EO) or alkyl sulfate (e.g. C ₁₆₋₁₈)	1	-	4%
	Alcohol ethoxylate (e.g. C ₁₄₋₁₅ alcohol, 7 EO)	5	-	9%
	Sodium carbonate (as Na ₂ CO ₃)	14	-	20%
25	Soluble silicate (as Na ₂ O, 2SiO ₂)	2	-	6%
	Zeolite (as NaAlSiO ₄)	15	-	22%
	Sodium sulfate (as Na ₂ SO ₄)	0	-	6%
	Sodium citrate/citric acid (as C ₆ H ₅ Na ₃ O ₇ /C ₆ H ₈ O ₇)	0	-	15%
30	Sodium perborate (as NaBO ₃ ·H ₂ O)	11	-	18%
	TAED	2	-	6%
	Carboxymethylcellulose	0	-	2%
	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0	-	3%
35	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
	Minor ingredients (e.g. suds suppressors, perfume, optical brightener, photobleach)	0	-	5%

2) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

5	Linear alkylbenzenesulfonate (calculated as acid)	6 - 11%
	Alcohol ethoxysulfate (e.g. C ₁₂₋₁₈ alcohol, 1-2 EO or alkyl sulfate (e.g. C ₁₆₋₁₈))	1 - 3%
10	Alcohol ethoxylate (e.g. C ₁₄₋₁₅ alcohol, 7 EO)	5 - 9%
	Sodium carbonate (as Na ₂ CO ₃)	15 - 21%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	1 - 4%
15	Zeolite (as NaAlSiO ₄)	24 - 34%
	Sodium sulfate (as Na ₂ SO ₄)	4 - 10%
	Sodium citrate/citric acid (as C ₆ H ₅ Na ₃ O ₇ /C ₆ H ₈ O ₇)	0 - 15%
	Carboxymethylcellulose	0 - 2%
20	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1 - 6%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
25	Minor ingredients (e.g. suds suppressors, perfume)	0 - 5%

3) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

30	Linear alkylbenzenesulfonate (calculated as acid)	5 - 9%
	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO)	7 - 14%
35	Soap as fatty acid (e.g. C ₁₆₋₂₂ fatty acid)	1 - 3%
	Sodium carbonate (as Na ₂ CO ₃)	10 - 17%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	3 - 9%
	Zeolite (as NaAlSiO ₄)	23 - 33%
	Sodium sulfate (as Na ₂ SO ₄)	0 - 4%
40	Sodium perborate (as NaBO ₃ ·H ₂ O)	8 - 16%

	TAED	2	-	8%
	Phosphonate (e.g. EDTMPA)	0	-	1%
	Carboxymethylcellulose	0	-	2%
5	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0	-	3%
	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
10	Minor ingredients (e.g. suds suppressors, perfume, optical brightener)	0	-	5%

4) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

15	Linear alkylbenzenesulfonate (calculated as acid)	8	-	12%
	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO)	10	-	25%
20	Sodium carbonate (as Na ₂ CO ₃)	14	-	22%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	1	-	5%
	Zeolite (as NaAlSiO ₄)	25	-	35%
	Sodium sulfate (as Na ₂ SO ₄)	0	-	10%
	Carboxymethylcellulose	0	-	2%
25	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1	-	3%
	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
30	Minor ingredients (e.g. suds suppressors, perfume)	0	-	5%

5) An aqueous liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	-	21%
35	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO or C ₁₂₋₁₅ alcohol, 5 EO)	12	-	18%
	Soap as fatty acid (e.g. oleic acid)	3	-	13%
40	Alkenylsuccinic acid (C ₁₂₋₁₄)	0	-	13%

	Aminoethanol	8	- 18%
	Citric acid	2	- 8%
	Phosphonate	0	- 3%
	Polymers (e.g. PVP, PEG)	0	- 3%
5	Borate (as B ₂ O ₃)	0	- 2%
	Ethanol	0	- 3%
	Propylene glycol	8	- 14%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
10	Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brightener)	0	- 5%

6) An aqueous structured liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	- 21%
20	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO, or C ₁₂₋₁₅ alcohol, 5 EO)	3	- 9%
	Soap as fatty acid (e.g. oleic acid)	3	- 10%
	Zeolite (as NaAlSiO ₄)	14	- 22%
	Potassium citrate	9	- 18%
25	Borate (as B ₂ O ₃)	0	- 2%
	Carboxymethylcellulose	0	- 2%
	Polymers (e.g. PEG, PVP)	0	- 3%
30	Anchoring polymers such as, e.g., lauryl methacrylate/acrylic acid copolymer; molar ratio 25:1; MW 3800	0	- 3%
	Glycerol	0	- 5%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
35	Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brighteners)	0	- 5%

7) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

	Fatty alcohol sulfate	5	- 10%
5	Ethoxylated fatty acid monoethanol- amide	3	- 9%
	Soap as fatty acid	0	- 3%
	Sodium carbonate (as Na_2CO_3)	5	- 10%
	Soluble silicate (as $\text{Na}_2\text{O}, 2\text{SiO}_2$)	1	- 4%
	Zeolite (as NaAlSiO_4)	20	- 40%
10	Sodium sulfate (as Na_2SO_4)	2	- 8%
	Sodium perborate (as $\text{NaBO}_3 \cdot \text{H}_2\text{O}$)	12	- 18%
	TAED	2	- 7%
	Polymers (e.g. maleic/acrylic acid copolymer, PEG)	1	- 5%
15	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. optical brightener, suds suppressors, per- fume)	0	- 5%

8) A detergent composition formulated as a granulate comprising

	Linear alkylbenzenesulfonate (calculated as acid)	8	- 14%
25	Ethoxylated fatty acid monoethanol- amide	5	- 11%
	Soap as fatty acid	0	- 3%
	Sodium carbonate (as Na_2CO_3)	4	- 10%
	Soluble silicate (as $\text{Na}_2\text{O}, 2\text{SiO}_2$)	1	- 4%
	Zeolite (as NaAlSiO_4)	30	- 50%
30	Sodium sulfate (as Na_2SO_4)	3	- 11%
	Sodium citrate (as $\text{C}_6\text{H}_5\text{Na}_3\text{O}_7$)	5	- 12%
	Polymers (e.g. PVP, maleic/acrylic acid copolymer, PEG)	1	- 5%
35	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. suds suppressors, perfume)	0	- 5%

9) A detergent composition formulated as a granulate comprising

	Linear alkylbenzenesulfonate (calculated as acid)	6	- 12%
	Nonionic surfactant	1	- 4%
5	Soap as fatty acid	2	- 6%
	Sodium carbonate (as Na_2CO_3)	14	- 22%
	Zeolite (as NaAlSiO_4)	18	- 32%
	Sodium sulfate (as Na_2SO_4)	5	- 20%
	Sodium citrate (as $\text{C}_6\text{H}_5\text{Na}_3\text{O}_7$)	3	- 8%
10	Sodium perborate (as $\text{NaBO}_3 \cdot \text{H}_2\text{O}$)	4	- 9%
	Bleach activator (e.g. NOBS or TAED)	1	- 5%
	Carboxymethylcellulose	0	- 2%
15	Polymers (e.g. polycarboxylate or PEG)	1	- 5%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. optical brightener, perfume)	0	- 5%

20

10) An aqueous liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	- 23%
25	Alcohol ethoxysulfate (e.g. C_{12-15} alcohol, 2-3 EO)	8	- 15%
	Alcohol ethoxylate (e.g. C_{12-15} al- cohol, 7 EO, or C_{12-15} alcohol, 5 EO)	3	- 9%
30	Soap as fatty acid (e.g. lauric acid)	0	- 3%
	Aminoethanol	1	- 5%
	Sodium citrate	5	- 10%
	Hydrotrope (e.g. sodium toluenesulfonate)	2	- 6%
35	Borate (as B_2O_3)	0	- 2%
	Carboxymethylcellulose	0	- 1%
	Ethanol	1	- 3%
	Propylene glycol	2	- 5%

	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
5	Minor ingredients (e.g. polymers, dispersants, perfume, optical brighteners)	0 - 5%

11) An aqueous liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	20 - 32%
10	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO, or C ₁₂₋₁₅ alcohol, 5 EO)	6 - 12%
	Aminoethanol	2 - 6%
	Citric acid	8 - 14%
15	Borate (as B ₄ O ₇)	1 - 3%
20	Polymer (e.g. maleic/acrylic acid copolymer, anchoring polymer such as, e.g., lauryl methacrylate/acrylic acid copolymer)	0 - 3%
	Glycerol	3 - 8%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
25	Minor ingredients (e.g. hydro-tropes, dispersants, perfume, optical brighteners)	0 - 5%

12) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

30	Anionic surfactant (linear alkylbenzenesulfonate, alkyl sulfate, alpha-olefinsulfonate, alpha-sulfo fatty acid methyl esters, alkanesulfonates, soap)	25 - 40%
35	Nonionic surfactant (e.g. alcohol ethoxylate)	1 - 10%
	Sodium carbonate (as Na ₂ CO ₃)	8 - 25%
	Soluble silicates (as Na ₂ O, 2SiO ₂)	5 - 15%
	Sodium sulfate (as Na ₂ SO ₄)	0 - 5%
40	Zeolite (as NaAlSiO ₄)	15 - 28%
	Sodium perborate (as NaBO ₃ ·4H ₂ O)	0 - 20%

Bleach activator (TAED or NOBS)	0 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. perfume, optical brighteners)	0 - 3%

13) Detergent formulations as described in 1) - 12) wherein all or part of the linear alkylbenzenesulfonate is replaced by (C₁₂-C₁₈) alkyl sulfate.

10

14) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

(C ₁₂ -C ₁₈) alkyl sulfate	9 - 15%
Alcohol ethoxylate	3 - 6%
Polyhydroxy alkyl fatty acid amide	1 - 5%
Zeolite (as NaAlSiO ₄)	10 - 20%
Layered disilicate (e.g. SK56 from Hoechst)	10 - 20%
Sodium carbonate (as Na ₂ CO ₃)	3 - 12%
Soluble silicate (as Na ₂ O, 2SiO ₂)	0 - 6%
Sodium citrate	4 - 8%
Sodium percarbonate	13 - 22%
TAED	3 - 8%
Polymers (e.g. polycarboxylates and PVP=)	0 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. optical brightener, photo bleach, perfume, suds suppressors)	0 - 5%

15) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

(C ₁₂ -C ₁₈) alkyl sulfate	4 - 8%
Alcohol ethoxylate	11 - 15%

	Soap	1	- 4%
	Zeolite MAP or zeolite A	35	- 45%
	Sodium carbonate (as Na ₂ CO ₃)	2	- 8%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	0	- 4%
5	Sodium percarbonate	13	- 22%
	TAED	1	- 8%
	Carboxymethyl cellulose	0	- 3%
	Polymers (e.g. polycarboxylates and PVP)	0	- 3%
10	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. optical brightener, phosphonate, perfume)	0	- 3%

15 16) Detergent formulations as described in 1) - 15) which contain a stabilized or encapsulated peracid, either as an additional component or as a substitute for already specified bleach systems.

20 17) Detergent compositions as described in 1), 3), 7), 9) and 12) wherein perborate is replaced by percarbonate.

18) Detergent compositions as described in 1), 3), 7), 9), 12), 14) and 15) which additionally contain a manganese catalyst.

25 The manganese catalyst may, e.g., be one of the compounds described in "Efficient manganese catalysts for low-temperature bleaching", Nature 362, 1994, pp. 637-639.

19) Detergent composition formulated as a nonaqueous detergent
30 liquid comprising a liquid nonionic surfactant such as, e.g., linear alkoxyated primary alcohol, a builder system (e.g. phosphate), enzyme and alkali. The detergent may also comprise anionic surfactant and/or a bleach system.

35 The α -amylase variant of the invention may be incorporated in concentrations conventionally employed in detergents. It is at present contemplated that, in the detergent composition of the invention, the α -amylase may be added in an amount correspon-

ding to 0.00001-1 mg (calculated as pure enzyme protein) of α -amylase per liter of wash liquor.

Dishwashing Composition

- 5 The dishwashing detergent composition comprises a surfactant which may be anionic, non-ionic, cationic, amphoteric or a mixture of these types. The detergent will contain 0-90% of non-ionic surfactant such as low- to non-foaming ethoxylated propoxylated straight-chain alcohols.
- 10 The detergent composition may contain detergent builder salts of inorganic and/or organic types. The detergent builders may be subdivided into phosphorus-containing and non-phosphorus-containing types. The detergent composition usually contains 1-90% of detergent builders.
- 15 Examples of phosphorus-containing inorganic alkaline detergent builders, when present, include the water-soluble salts especially alkali metal pyrophosphates, orthophosphates, and polyphosphates. An example of phosphorus-containing organic alkaline detergent builder, when present, includes the water-
- 20 soluble salts of phosphonates. Examples of non-phosphorus-containing inorganic builders, when present, include water-soluble alkali metal carbonates, borates and silicates as well as the various types of water-insoluble crystalline or amorphous alumino silicates of which zeolites are the best-known
- 25 representatives.

Examples of suitable organic builders include the alkali metal, ammonium and substituted ammonium, citrates, succinates, malonates, fatty acid sulphonates, carboxymethoxy succinates,

30 ammonium polyacetates, carboxylates, polycarboxylates, amino-polycarboxylates, polyacetyl carboxylates and polyhydroxysulphonates.

Other suitable organic builders include the higher molecular

35 weight polymers and co-polymers known to have builder properties, for example appropriate polyacrylic acid, polymaleic and polyacrylic/polymaleic acid copolymers and their salts.

The dishwashing detergent composition may contain bleaching agents of the chlorine/bromine-type or the oxygen-type. Examples of inorganic chlorine/bromine-type bleaches are lithium, sodium or calcium hypochlorite and hypobromite as well
5 as chlorinated trisodium phosphate. Examples of organic chlorine/bromine-type bleaches are heterocyclic N-bromo and N-chloro imides such as trichloroisocyanuric, tribromoisocyanuric, dibromoisocyanuric and dichloroisocyanuric acids, and salts thereof with water-solubilizing cations such as potassium
10 and sodium. Hydantoin compounds are also suitable.

The oxygen bleaches are preferred, for example in the form of an inorganic persalt, preferably with a bleach precursor or as a peroxy acid compound. Typical examples of suitable peroxy
15 bleach compounds are alkali metal perborates, both tetrahydrates and monohydrates, alkali metal percarbonates, persilicates and perphosphates. Preferred activator materials are TAED and glycerol triacetate.

20 The dishwashing detergent composition of the invention may be stabilized using conventional stabilizing agents for the enzyme(s), e.g. a polyol such as e.g. propylene glycol, a sugar or a sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g. an aromatic borate ester.

25

The dishwashing detergent composition of the invention may also contain other conventional detergent ingredients, e.g. deflocculant material, filler material, foam depressors, anti-corrosion agents, soil-suspending agents, sequestering agents,
30 anti-soil redeposition agents, dehydrating agents, dyes, bactericides, fluorescers, thickeners and perfumes.

Finally, the α -amylase variant of the invention may be used in conventional dishwashing detergents, e.g. in any of the
35 detergents described in any of the following patent publications:

EP 518719, EP 518720, EP 518721, EP 516553, EP 516554,

EP 516555, GB 2200132, DE 3741617, DE 3727911, DE 4212166,
DE 4137470, DE 3833047, WO 93/17089, DE 4205071, WO 52/09680,
WO 93/18129, WO 93/04153, WO 92/06157, WO 92/08777, EP 429124,
WO 93/21299, US 5141664, EP 561452, EP 561446, GB 2234980,
5 WO 93/03129, EP 481547, EP 530870, EP 533239, EP 554943,
EP 346137, US 5112518, EP 318204, EP 318279, EP 271155,
EP 271156, EP 346136, GB 2228945, CA 2006687, WO 93/25651,
EP 530635, EP 414197, US 5240632.

10 EXAMPLES

EXAMPLE 1

15 Example on Homology building of TERM

The overall homology of the *B. licheniformis* α -amylase (in the following referred to as TERM) to other Termamyl-like α -amylases is high and the percent similarity is extremely high.
20 The similarity calculated for TERM to BSG (the *B. stearothermophilus* α -amylase with SEQ ID NO 6), and BAN (the *B. amyloliquefaciens* α -amylase with SEQ ID NO 4) using the University of Wisconsin Genetics Computer Group's program GCG gave 89% and 78%, respectively. TERM has a deletion of 2
25 residues between residue G180 and K181 compared to BAN and BSG. BSG has a deletion of 3 residues between G371 and I372 in comparison with BAN and TERM. Further BSG has a C-terminal extension of more than 20 residues compared to BAN and TERM. BAN has 2 residues less and TERM has one residue less in the
30 N-terminal compared to BSG.

The structure of the *B. licheniformis* (TERM) and of the *B. amyloliquefaciens* α -amylase (BAN), respectively, was model built on the structure disclosed in Appendix 1 herein. The
35 structure of other Termamyl-like α -amylases (e.g. those disclosed herein) may be built analogously.

In comparison with the α -amylase used for elucidating the present structure, TERM differs in that it lacks two residues around 178-182. In order to compensate for this in the model structure, the HOMOLOGY program from BIOSYM was used to substitute the residues in equivalent positions in the structure (not only structurally conserved regions) except for the deletion point. A peptide bond was established between G179(G177) and K180(K180) in TERM(BAN). The close structural relationship between the solved structure and the model structure (and thus the validity of the latter) is indicated by the presence of only very few atoms found to be too close together in the model.

To this very rough structure of TERM was then added all waters (605) and ions (4 Calcium and 1 Sodium) from the solved structure (Appendix 1) at the same coordinates as for said solved structure using the INSIGHT program. This could be done with only few overlaps - in other words with a very nice fit. This model structure were then minimized using 200 steps of Steepest descent and 600 steps of Conjugated gradient (see Brooks et al 1983, J. Computational Chemistry 4, p.187-217). The minimized structure was then subjected to molecular dynamics, 5ps heating followed by up to 200ps equilibration but more than 35ps. The dynamics as run with the Verlet algorithm and the equilibration temperature 300K were kept using the Berendsen coupling to a waterbath (Berendsen et. al., 1984, J. Chemical Physics 81, p. 3684-3690). Rotations and translations were removed every picosecond. The potential energy became stable after appr. 35ps equilibration. A mean dynamics structure was extracted and can be used for further analysis.

EXAMPLE 2

Determination of residues within 10Å from the ions present in the solved structure

The coordinates of Appendix 1 are read into the INSIGHT program provided by BIOSYM technologies. The spatial coordinates are

presented showing the bonds between the atoms. The ions are presented as well as the water atoms. The program package part of creating subset are used to create a 10Å subset around the Calcium and the Sodium ions in the structure using the command
5 ZONE. All residues having an atom within the 10Å are compiled and written out by the LIST MOLECULE command. By giving the ions the name ium in the coordinate file a 10Å sphere around all atoms called ium is compiled. The specific residues identified in this manner are given further above in the
10 section entitled "Ca²⁺ dependency".

EXAMPLE 3

Determination of cavities in the solved structure (Appendix 1)

15

The solved structure exhibits many internal holes and cavities. When analysing for such cavities the Connolly program is normally used (Lee, B. and Richards, F.M. (1971) J. Mol. Biol. 55,p. 379-400). The program uses a probe with radius to search
20 the external and internal surface of the protein. The smallest hole observable in this way has the probe radius.

To analyse the solved structure a modified version of the Connolly program included in the program of INSIGHT were used.
25 First the water molecules and the ions were removed by unmerging these atoms from the solved structure. By using the command MOLECULE SURFACE SOLVENT the solvent accessible surface area were calculated for all atoms and residues using a probe radius of 1.4Å, and displayed on the graphics screen together
30 with the model of the solved structure. The internal cavities where then seen as dot surfaces with no connections to external surface.

Mutant suggestions for filling out the holes are given in the
35 specification (in the section entitled "Variants with increased thermostability and/or altered temperature optimum"). By using the homology build structures or/and the sequence alignment

mutations for the homologous structures of TERM and BSG and BAN can be made.

EXAMPLE 4

5

Construction of Termamyl™ variants in accordance with the invention

Termamyl (SEQ ID NO. 2) is expressed in *B. subtilis* from a
10 plasmid denoted pDN1528. This plasmid contains the complete
gene encoding Termamyl, *amyL*, the expression of which is
directed by its own promoter. Further, the plasmid contains the
origin of replication, *ori*, from plasmid pUB110 and the *cat*
gene from plasmid pC194 conferring resistance towards
15 chloramphenicol. pDN1528 is shown in Fig. 9.

A specific mutagenesis vector containing a major part of the
coding region of SEQ ID NO 1 was prepared. The important
features of this vector, denoted pJeEN1, include an origin of
20 replication derived from the pUC plasmids, the *cat* gene
conferring resistance towards chloramphenicol, and a
frameshift-containing version of the *bla* gene, the wild type of
which normally confers resistance towards ampicillin (*amp^R*
phenotype). This mutated version results in an *amp^S* phenotype.
25 The plasmid pJeEN1 is shown in Fig. 10, and the *E. coli* origin
of replication, *ori*, *bla*, *cat*, the 5'-truncated version of the
Termamyl amylase gene, and selected restriction sites are
indicated on the plasmid.

30 Mutations are introduced in *amyL* by the method described by
Deng and Nickoloff (1992, Anal. Biochem. 200, pp. 81-88) except
that plasmids with the "selection primer" (primer #6616; see
below) incorporated are selected based on the *amp^R* phenotype of
transformed *E. coli* cells harboring a plasmid with a repaired
35 *bla* gene, instead of employing the selection by restriction
enzyme digestion outlined by Deng and Nickoloff. Chemicals and
enzymes used for the mutagenesis were obtained from the

Chameleon™ mutagenesis kit from Stratagene (catalogue number 200509).

After verification of the DNA sequence in variant plasmids, the truncated gene, containing the desired alteration, is subcloned into pDN1528 as a *Pst*I-*Eco*RI fragment and transformed into a protease- and amylase-depleted *Bacillus subtilis* strain in order to express the variant enzyme.

- 10 The Termamyl variant V54W was constructed by the use of the following mutagenesis primer (written 5' to 3', left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CGC TTG

- 15 The Termamyl variant A52W + V54W was constructed by the use of the following mutagenesis primer (written 5' to 3', left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CCA TTG GCT CG

20

Primer #6616 (written 5' to 3', left to right; P denotes a 5' phosphate):

P CTG TGA CTG GTG AGT ACT CAA CCA AGT C

25

EXAMPLE 5

Saccharification in the presence of "residual" α -amylase activity

30

Two appropriate Termamyl variants with altered specificity were evaluated by saccharifying a DE 10 (DE = dextrose equivalent) maltodextrin substrate with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase under conditions where the variant amylase was active.

Saccharification: Substrates for saccharification were prepared by dissolving 230 g DE 10 spray-dried maltodextrin, prepared

from common corn starch, in 460 ml boiling deionized water and adjusting the dry substance (DS) content to approximately 30% w/w. The pH was adjusted to 4.7 (measured at 60°C) and aliquots of substrate corresponding to 15 g dry weight were transferred to 50 ml blue cap glass flasks.

The flasks were then placed in a shaking water bath equilibrated at 60°C, and the enzymes added. The pH was readjusted to 4.7 where necessary.

10

The following enzymes were used:

Glucoamylase: AMG™ (Novo Nordisk A/S); dosage 0.18 AG/g DS

Pullulanase: Promozyme™ (Novo Nordisk A/S);

15 dosage 0.06 PUN/g DS

α-Amylases: Termamyl™ (Novo Nordisk A/S); dosage 60 NU/g DS

Termamyl variant V54W; dosage 60 NU/g DS

Termamyl variant V54W + A52W; dosage 60 NU/g DS

20 2 ml samples were taken periodically. The pH of each sample was adjusted to about 3.0, and the sample was then heated in a boiling water bath for 15 minutes to inactivate the enzymes. After cooling, the samples were treated with approximately 0.1 g mixed-bed ion exchange resin (BIO-Rad 501-X (D)) for 30 minutes on a rotary mixer and then filtered. The carbohydrate composition of each sample was determined by HPLC. The following results were obtained after 72 hours [DP_n denotes a dextrose (D-glucose) oligomer with n glucose units]:

30

α-amylase	%DP ₁	%DP ₂	%DP ₃	%DP ₄
None (control)	95.9	2.8	0.4	1.0
V54W	96.0	2.9	0.4	0.8
35 V54W + A52W	95.9	2.8	0.4	0.8
Termamyl™	95.6	2.8	0.8	0.8

It can be seen from the above results that compared with the control (no α -amylase activity present during liquefaction), the presence of α -amylase activity from variants V54W and V54W + A52W did not lead to elevated panose (DP₃) levels. In contrast, Termamyl α -amylase activity resulted in higher levels of panose and a subsequent loss of D-glucose (DP₁) yield.

Thus, if α -amylase variants V54W or V54W + A52W are used for starch liquefaction, it will not be necessary to inactivate the residual α -amylase activity before the commencement of saccharification.

EXAMPLE 6

15 Calcium-binding affinity of α -amylase variants of the invention

Unfolding of amylases by exposure to heat or to denaturants such as guanidine hydrochloride is accompanied by a decrease in fluorescence. Loss of calcium ions leads to unfolding, and the affinity of α -amylases for calcium can be measured by fluorescence measurements before and after incubation of each α -amylase (e.g. at a concentration of 10 μ g/ml) in a buffer (e.g. 50 mM HEPES, pH 7) with different concentrations of calcium (e.g. in the range of 1 μ M-100 mM) or of EGTA (e.g. in the range of 1-1000 μ M) [EGTA = 1,2-di(2-aminoethoxy)ethane-N,N,N',N'-tetraacetic acid] for a sufficiently long period of time (such as 22 hours at 55°C).

The measured fluorescence F is composed of contributions from the folded and unfolded forms of the enzyme. The following equation can be derived to describe the dependence of F on calcium concentration ($[Ca]$):

$$F = [Ca]/(K_{diss} + [Ca])(\alpha_N - \beta_N \log([Ca])) + K_{diss}/(K_{diss} + [Ca])(\alpha_U - \beta_U \log([Ca]))$$

where α_N is the fluorescence of the native (folded) form of the enzyme, β_N is the linear dependence of α_N on the logarithm of

the calcium concentration (as observed experimentally), α_u is the fluorescence of the unfolded form and β_u is the linear dependence of α_u on the logarithm of the calcium concentration. K_{diss} is the apparent calcium-binding constant for an equilibrium process as follows:



10 In fact, unfolding proceeds extremely slowly and is irreversible. The rate of unfolding is dependent on calcium concentration, and the dependency for a given α -amylase provides a measure of the Ca-binding affinity of the enzyme. By defining a standard set of reaction conditions (e.g. 22 hours
15 at 55°C), a meaningful comparison of K_{diss} for different α -amylases can be made. The calcium dissociation curves for α -amylases in general can be fitted to the equation above, allowing determination of the corresponding values of K_{diss} .

20 The following values for K_{diss} were obtained for a parent Termamyl-like α -amylase having the amino acid sequence shown in SEQ ID No. 1 of WO 95/26397 and for the indicated variant thereof according to the invention:

25 α -Amylase	K_{diss} (mol/l)
L351C + M430C + T183* + G184*	$1.7 (\pm 0.5) \times 10^{-3}$
Parent	$3.5 (\pm 1.1) \times 10^{-1}$

30

It is apparent from the above that the calcium-binding affinity of the variant in question binds calcium significantly more strongly than the parent, and thereby has a correspondingly lower calcium dependency than the parent.

35

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SEQUENCE LISTING

In the following SEQ ID Nos. 1, 3, 5 the 5', coding sequence and 3' sequence of the relevant α -amylase genes are illustrated. The 5' sequence is the first separate part of the sequence written with lower case letters, the coding sequence is the intermediate part of the sequence, where the signal sequence is written with lower case letters and the sequence encoding the mature α -amylase is written with upper case letters, and the 3' sequence is the third separate part of the sequence written with lower case letters.

SEQ ID No. 1

15

cggaagattggaagtacaaaaataagcaaaagattgtcaatcatgtcatgagccatgcgg-
gagacggaaaaatcgtctta atgcacgatatttatgcaacgttcgcagatgctgctgaa-
gagattattaaaaagctgaaagcaaaaggctatcaattggt aactgtatctcagcttga-
agaagtgaagaagcagagaggctattgaataaatgagtagaagcgccatatcggcgcttttc
20 ttttggaagaaaatatagggaaaatggtacttggttaaaaattcgggaatatttataacaacatc-
atatgtttcacattgaaa ggggaggagaatc

atgaaacaacaaaaacggctttacgcccgattgctgacgctgttatttgcgctcatcttctt-
gctgc ctcattctgcagcagcgcgGCAAATCTTAATGGGACGCTGATGCAGTATTTT-
25 GAATGGTACATGCCCAATGACGGCCAA CATTGGAGGCGTTTGCAAAACGACTCGGCATAT-
TTGGCTGAACACGGTATTACTGCCGTCTGGATTCCCCCGGCATATAA GGGAACGAGC-
CAAGCGGATGTGGGCTACGGTGCTTACGACCTTTATGATTTAGGGGAGTTTCATCAAAAAG-
GGACGGTTC GGACAAAGTACGGCACAAAAGGAGAGCTGCAATCTGCGATCAAAAGTCTTC-
ATTCCCGCGACATTAACGTTTACGGGGAT GTGGTCATCAACCACAAAGGCGGCGCTGA-
30 TGCGACCGAAGATGTAACCGCGGTTGAAGTCGATCCCGCTGACCGCAACCG CGTAATTT-
CAGGAGAACACCTAATTAAAGCCTGGACACATTTTTCATTTTCCGGGGCGCGGCAGCACATA-
CAGCGATTTTA AATGGCATTGGTACCATTTTGACGGAACCGATTGGGACGAGTCCCGAAA-
GCTGAACCGCATCTATAAGTTTCAAGGAAAG GCTTGGGATTGGGAAGTTTCCAATGAA-
AACGGCAACTATGATTATTTGATGTATGCCGACATCGATTATGACCATCCTGA TGTCGCAG-
35 CAGAAATTAAGAGATGGGGCACTTGGTATGCCAATGAACTGCAATTGGACGGTTTCCGTCTT-
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AAAAACGGGGAAGGAAATGTTTACGGTAGCT GAATATTGGCAGAAT-
GACTTGGGCGCGCTGGAAAACCTATTTGAACAAAACAAATTTTAATCATTGAGTGTGAC-

GTGCC GCTTCATTATCAGTTCCATGCTGCATCGACACAGGGAGGCGGCTATGATATGAG-
GAAATTGCTGAACGGTACGGTCGTTT CCAAGCATCCGTTGAAATCGGTTACATTTGTCG-
ATAACCATGATACACAGCCGGGGCAATCGCTTGAGTCGACTGTCCAA ACATGGTTTAAG-
CCGCTTGCTTACGCTTTTATTCTCACAAGGGAATCTGGATACCCTCAGGTTTTCTACGGG-
5 GATATGTA CGGGACGAAAGGAGACTCCCAGCGCGAAATTCCTGCCTTGAAACACAAAAT-
TGAACCGATCTTAAAAGCGAGAAAACAGT ATGCGTACGGAGCACAGCATGATTATTTGAC-
CACCATGACATTGTCCGCTGGACAAGGGAAGGCGACAGCTCGGTTGCA AATTCAGGTTTGG-
CGGCATTAATAACAGACGGACCCGGTGGGGCAAAGCGAATGTATGTCCGCCGGCA-
AAACGCCGGTGA GACATGGCATGACATTACCGGAAACCGTTCGGAGCCGGTTGTCATCA-
10 ATTCGGAAGGCTGGGGAGAGTTTCACGTAAACG GCGGGTCGGTTTCAATTTATGTTCAA-
GATAG

aagagcagagaggacggatttcctgaaggaaatccggtttttttat

15 SEQ ID No. 2

ANLNGTLMQYFEWYMPNDGQHWRRLLQND SAYLAEHGITAV
WIPPAYKGTSQADVGYGAYDLYDLGEFHQKGTVRTKYGTK
GELQSAIKSLHSRDINVYGDVVINHKGGADATEDVTAVEV
20 DPADRN RVISGEHLIKAWTHFHFPGRGSTYSDFKWHWYHF
DGTDWDESRLNRIYKFQKAWDWEVSNENGN DYLYMYAD
IDYDHPDVAAEIKRWGTWYANELQLDGFRLDAVKHIKFSF
LRDWNHVRKGTGKEMFTVAEYWQNDLGALENYLNKTNFN
HSVFDVPLHYQFHAASQTGGGYDMRKLNGTVVSKHPLKS
25 VTFVDNHDTQPGQSLESTVQTFKPLAYAFILTRESGYPO
VFYGD MYGTGDSQREIPALKHKIEPILKARKQYAYGAQH
DYFDHHDIVGWTREGDSSVANSGLAALITDGPGGAKRMYV
GRQNAGETWHDITGNRSEPVVINSEGWGEFHVNGGSVSIY
VQR

30

SEQ ID No. 3

gccccgcacatacgaaaagactggctgaaaacattgagcctttgatgactgatgatttgg-
35 ctgaagaagtggatcgattg tttgagaaaagaagaagaccataaaaaataccttgtctgt-
catcagacaggggtattttttatgctgtccagactgtccgct gtgtaaaaaataaggaata-
aaggggggttgttatttttactgatatgtaaaatataatttgtataagaaaatgagaggg
agaagaaac

atgattcaaaaacgaaagcggacagtttcggtcagacttggtgcttatgtgcacgctggtt-
atgtgtcagttt gccgattacaaaaacatcagccGTAAATGGCACGCTGATGCAGTATT-
TTGAATGGTATACGCCGAACGACGGCCAGCATT GGAAACGATTGCAGAATGATGCGGAA-
CATTATCGGATATCGGAATCACTGCCGTCTGGATTCCCTCCCGCATACAAAGGA TTGAG-
5 CCAATCCGATAACGGATACGGACCTTATGATTTGTATGATTTAGGAGAATTCCAGCAAAA-
AGGGACGGTCAGAAC GAAATACGGCACAAAATCAGAGCTTCAAGATGCGATCGGCTCAC-
TGCATTCCCGGAACGTCCAAGTATACGGAGATGTGG TTTTGAATCATAAGGCTGGTGCT-
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SEQ ID No. 4

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10 QSVFDVPLHFNLQAASSQGGGYDMRRLLDGTVVSRHPEKA
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15

SEQ ID No. 5

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15

SEQ ID No. 6

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SEQ ID No. 10

35 1 ATPADWRSQS IYFLLTDRFA RTDGSTTATC
31 NTADQKYCGG TWQGIIDKLD YIQGMGFTAI
61 WITPVTAQLP QTTAYGDAYH GYWQQDIYSL
91 NENYGTADDL KALSSALHER GMYLMVDVVA

121 NHMGYDGAGS SVDYSVFKPF SSQDYFHPFC
151 FIQNYEDQTQ VEDCWLGDNT VSLPDLDTTK
181 DVVKNEWYDW VGSLVSNYSI DGLRIDTVKH
211 VQKDFWPGYN KAAGVYCIGE VLDGDPAYTC
5 241 PYQNVMDGVL NYPIYYPLLN AFKSTSGSMD
271 DLYNMINTVK SDCPDSTLLG TFVENHDNPR
301 FASYTNDIAL AKNVAAFIIL NDGIPIIYAG
331 QEQHYAGGND PANREATWLS GYPTDSELYK
361 LIASANAIRN YAISKDTGFV TYKNWPIYKD
10 391 DITIAMRKGT DGSQIVTILS NKGASGDSYT
421 LSLSGAGYTA GQQLTEVIGC TTVTVGSDGN
451 VPVPMAGGLP RVLYPTEKLA GSKICSSS

ATOM	1	CB	VAL A	1	11.902	27.157	22.095	1.00	23.86	6	ATOM	54	CB	TYR A	8	28.238	37.382	24.476	1.00	10.19	6
ATOM	2	CG1	VAL A	1	12.302	27.494	22.658	1.00	24.08	6	ATOM	55	CG	TYR A	8	27.909	38.377	23.351	1.00	10.76	6
ATOM	3	CG2	VAL A	1	10.659	27.948	22.511	1.00	26.37	6	ATOM	56	CD	TYR A	8	27.180	37.983	22.222	1.00	11.00	6
ATOM	4	C	VAL A	1	13.030	25.096	22.743	1.00	19.54	6	ATOM	57	CE1	TYR A	8	26.891	38.842	21.190	1.00	11.22	6
ATOM	5	O	VAL A	1	13.191	25.013	23.967	1.00	19.86	8	ATOM	58	CD2	TYR A	8	28.340	39.698	23.424	1.00	10.96	6
ATOM	6	N	VAL A	1	10.702	25.241	23.415	1.00	20.28	7	ATOM	59	CE2	TYR A	8	28.080	40.620	22.423	1.00	11.25	6
ATOM	7	CA	VAL A	1	11.659	25.658	22.335	1.00	20.25	6	ATOM	60	CZ	TYR A	8	27.358	40.156	21.312	1.00	11.62	6
ATOM	8	N	ASH A	2	13.867	24.729	21.802	1.00	18.39	7	ATOM	61	OH	TYR A	8	27.114	41.063	20.294	1.00	11.87	8
ATOM	9	CA	ASH A	2	15.168	24.197	22.212	1.00	16.73	6	ATOM	62	C	TYR A	8	30.789	37.289	24.119	1.00	9.70	6
ATOM	10	CB	ASH A	2	15.836	23.657	20.945	1.00	16.09	6	ATOM	63	O	TYR A	8	30.918	38.427	24.563	1.00	9.67	8
ATOM	11	CG	ASH A	2	15.219	22.336	20.451	1.00	15.33	6	ATOM	64	N	PHE A	9	31.890	36.710	23.639	1.00	9.16	7
ATOM	12	OO1	ASH A	2	14.707	21.549	21.252	1.00	15.28	8	ATOM	65	CA	PHE A	9	33.191	37.307	23.588	1.00	9.15	6
ATOM	13	HD2	ASH A	2	15.283	22.082	19.151	1.00	12.41	7	ATOM	66	CB	PHE A	9	33.805	37.750	24.941	1.00	8.08	6
ATOM	14	C	ASH A	2	15.969	25.334	22.787	1.00	15.71	6	ATOM	67	CG	PHE A	9	33.968	36.659	25.978	1.00	9.21	6
ATOM	15	O	ASH A	2	15.903	26.435	22.198	1.00	16.02	8	ATOM	68	CD1	PHE A	9	35.239	36.125	26.240	1.00	10.15	6
ATOM	16	N	GLY A	3	16.720	25.198	23.833	1.00	14.56	7	ATOM	69	CD2	PHE A	9	32.887	36.171	26.720	1.00	7.79	6
ATOM	17	CA	GLY A	3	17.541	26.305	24.331	1.00	13.21	6	ATOM	70	CE1	PHE A	9	35.440	35.161	27.245	1.00	10.23	6
ATOM	18	C	GLY A	3	18.940	26.211	23.671	1.00	12.14	6	ATOM	71	CE2	PHE A	9	33.070	35.205	27.669	1.00	7.66	6
ATOM	19	O	GLY A	3	19.498	25.153	23.302	1.00	11.92	8	ATOM	72	CZ	PHE A	9	34.313	34.698	27.962	1.00	8.17	6
ATOM	20	N	THR A	4	19.503	27.368	23.499	1.00	11.28	7	ATOM	73	C	PHE A	9	34.173	36.294	22.963	1.00	8.94	6
ATOM	21	CA	THR A	4	20.829	27.555	22.912	1.00	10.96	6	ATOM	74	O	PHE A	9	33.903	35.102	22.918	1.00	8.63	8
ATOM	22	CB	THR A	4	20.721	27.878	21.400	1.00	11.09	6	ATOM	75	N	GLU A	10	35.284	36.856	22.536	1.00	9.09	7
ATOM	23	OG1	THR A	4	19.920	26.828	20.782	1.00	12.31	8	ATOM	76	CA	GLU A	10	36.430	36.089	22.006	1.00	9.38	6
ATOM	24	CG2	THR A	4	22.048	27.933	20.693	1.00	8.99	6	ATOM	77	CB	GLU A	10	36.508	36.043	20.513	1.00	7.45	6
ATOM	25	C	THR A	4	21.584	28.664	23.663	1.00	10.56	6	ATOM	78	CG	GLU A	10	37.604	37.345	19.740	1.00	7.55	6
ATOM	26	O	THR A	4	21.080	29.743	23.866	1.00	9.98	8	ATOM	79	CD	GLU A	10	37.981	37.580	19.156	1.00	6.81	6
ATOM	27	N	LEU A	5	22.809	28.376	24.092	1.00	10.63	7	ATOM	80	OE1	GLU A	10	38.145	38.544	18.397	1.00	8.43	8
ATOM	28	CA	LEU A	5	23.700	29.291	24.818	1.00	10.69	6	ATOM	81	OE2	GLU A	10	38.962	36.877	19.438	1.00	5.00	8
ATOM	29	CB	LEU A	5	24.515	28.477	25.789	1.00	9.46	6	ATOM	82	C	GLU A	10	37.636	36.715	22.737	1.00	9.90	6
ATOM	30	CG	LEU A	5	25.429	28.946	26.864	1.00	10.96	6	ATOM	83	O	GLU A	10	37.590	37.807	23.361	1.00	9.92	8
ATOM	31	CD1	LEU A	5	24.887	30.150	27.608	1.00	9.46	6	ATOM	84	N	TRP A	11	38.791	36.059	22.729	1.00	10.15	7
ATOM	32	CD2	LEU A	5	25.608	27.802	27.884	1.00	10.55	6	ATOM	85	CA	TRP A	11	39.980	36.551	23.407	1.00	10.35	6
ATOM	33	C	LEU A	5	24.644	29.992	23.840	1.00	10.85	6	ATOM	86	CB	TRP A	11	42.271	35.940	24.181	1.00	11.61	6
ATOM	34	O	LEU A	6	25.047	29.453	22.799	1.00	10.88	8	ATOM	87	CG	TRP A	11	41.182	35.619	23.186	1.00	9.98	6
ATOM	35	N	MET A	6	25.031	31.217	24.123	1.00	10.80	7	ATOM	88	CD2	TRP A	11	42.292	35.583	25.565	1.00	12.44	6
ATOM	36	CA	MET A	6	25.971	31.930	23.312	1.00	10.94	6	ATOM	89	CE2	TRP A	11	43.516	36.063	26.103	1.00	12.84	6
ATOM	37	CB	MET A	6	25.455	33.143	22.507	1.00	12.97	6	ATOM	90	CE3	TRP A	11	41.412	34.916	26.432	1.00	13.39	6
ATOM	38	CG	MET A	6	26.629	33.643	21.638	1.00	15.17	6	ATOM	91	CD1	TRP A	11	43.446	36.606	23.915	1.00	11.78	6
ATOM	39	SD	MET A	6	26.027	34.680	20.185	1.00	19.39	16	ATOM	92	ME1	TRP A	11	44.188	36.673	25.083	1.00	12.99	7
ATOM	40	CE	MET A	6	27.525	35.144	19.516	1.00	16.94	6	ATOM	93	CZ2	TRP A	11	43.831	35.890	27.441	1.00	13.37	6
ATOM	41	C	MET A	6	27.089	32.485	24.223	1.00	10.67	6	ATOM	94	CZ3	TRP A	11	41.717	34.763	27.772	1.00	13.91	6
ATOM	42	O	MET A	6	26.774	33.206	25.170	1.00	10.51	8	ATOM	95	CH2	TRP A	11	42.946	35.256	28.280	1.00	14.23	6
ATOM	43	N	GLN A	7	28.325	32.133	23.911	1.00	10.34	7	ATOM	96	C	TRP A	11	40.410	37.937	22.933	1.00	10.57	6
ATOM	44	CA	GLN A	7	30.696	31.910	24.617	1.00	10.20	6	ATOM	97	O	TRP A	11	40.843	38.709	23.797	1.00	10.67	8
ATOM	45	CB	GLN A	7	33.280	32.727	25.053	1.00	10.26	6	ATOM	98	N	TYR A	12	40.322	38.209	21.623	1.00	10.73	7
ATOM	46	CG	GLN A	7	31.967	32.632	25.053	1.00	10.26	6	ATOM	99	CA	TYR A	12	40.766	39.508	21.126	1.00	11.11	6
ATOM	47	CD	GLN A	7	33.280	31.914	25.027	1.00	9.15	6	ATOM	100	CB	TYR A	12	41.559	39.432	19.708	1.00	11.11	6
ATOM	48	OE2	GLN A	7	34.327	32.470	25.449	1.00	12.35	8	ATOM	101	CG	TYR A	12	42.765	38.515	20.029	1.00	11.60	6
ATOM	49	N	GLN A	7	33.359	30.714	24.570	1.00	6.58	7	ATOM	102	CD1	TYR A	12	42.605	37.158	19.704	1.00	11.95	6
ATOM	50	C	GLN A	7	29.578	34.125	24.015	1.00	10.22	6	ATOM	103	CE1	TYR A	12	43.666	36.268	19.892	1.00	12.43	6
ATOM	51	O	GLN A	7	29.856	34.167	22.786	1.00	10.30	8	ATOM	104	CD2	TYR A	12	43.985	38.951	20.540	1.00	11.88	6
ATOM	52	N	TYR A	8	29.394	35.236	24.691	1.00	9.97	7	ATOM	105	CE2	TYR A	12	45.023	38.076	20.714	1.00	11.85	6
ATOM	53	CA	TYR A	8	29.467	36.526	24.022	1.00	9.95	6	ATOM	106	CZ	TYR A	12	44.870	36.749	20.388	1.00	12.61	6

ATOM	107	OH	TYR A	12	45.854	35.787	20.560	1.00	13.18	8	ATOM	160	ME2	HIS A	19	31.584	41.112	24.073	1.00	9.42	7
ATOM	108	C	TYR A	12	39.687	40.574	20.991	1.00	11.38	6	ATOM	161	C	HIS A	19	30.007	45.489	25.132	1.00	9.04	6
ATOM	109	O	TYR A	12	39.862	41.436	20.132	1.00	11.53	8	ATOM	162	O	HIS A	19	29.153	44.838	24.493	1.00	8.75	8
ATOM	110	H	THR A	13	38.630	40.547	21.783	1.00	11.49	7	ATOM	163	H	TRP A	20	29.650	46.184	26.217	1.00	9.17	7
ATOM	111	CA	THR A	13	37.651	41.656	21.700	1.00	11.50	6	ATOM	164	CA	TRP A	20	28.248	46.090	26.688	1.00	9.56	6
ATOM	112	CB	THR A	13	36.604	41.321	22.761	1.00	13.32	6	ATOM	165	CB	TRP A	20	28.200	46.691	28.093	1.00	8.24	6
ATOM	113	CG1	THR A	13	35.755	40.296	22.169	1.00	14.85	8	ATOM	166	CG	TRP A	20	29.112	46.119	29.122	1.00	7.50	6
ATOM	114	CG2	THR A	13	35.732	42.466	23.175	1.00	14.00	6	ATOM	167	CG2	TRP A	20	29.515	44.774	29.341	1.00	7.46	6
ATOM	115	C	THR A	13	38.489	42.880	22.036	1.00	11.41	6	ATOM	168	CE2	TRP A	20	30.376	44.751	30.459	1.00	7.35	6
ATOM	116	O	THR A	13	39.429	42.805	22.840	1.00	11.13	8	ATOM	169	CE3	TRP A	20	29.187	43.568	28.695	1.00	8.23	6
ATOM	117	H	PRO A	14	38.254	44.015	21.408	1.00	11.47	7	ATOM	170	CD1	TRP A	20	29.736	46.854	30.088	1.00	7.37	6
ATOM	118	CD	PRO A	14	37.184	44.144	20.397	1.00	11.68	6	ATOM	171	ME1	TRP A	20	30.483	46.041	30.920	1.00	7.58	7
ATOM	119	CA	PRO A	14	38.979	45.243	21.811	1.00	11.44	6	ATOM	172	CE2	TRP A	20	30.926	43.591	31.006	1.00	6.78	6
ATOM	120	CB	PRO A	14	38.477	46.296	20.569	1.00	11.60	6	ATOM	173	CH3	TRP A	20	29.750	42.407	29.223	1.00	9.26	6
ATOM	121	CG	PRO A	14	37.352	45.564	19.896	1.00	11.77	6	ATOM	174	CH2	TRP A	20	30.608	42.427	30.366	1.00	7.69	6
ATOM	122	C	PRO A	14	38.706	45.868	22.993	1.00	11.21	6	ATOM	175	C	TRP A	20	27.227	46.746	25.757	1.00	9.73	6
ATOM	123	O	PRO A	14	37.703	45.785	23.618	1.00	11.15	8	ATOM	176	O	TRP A	20	26.070	46.395	25.592	1.00	9.42	8
ATOM	124	H	ASN A	15	39.806	46.557	23.445	1.00	10.84	7	ATOM	177	N	LYS A	21	27.591	47.832	25.102	1.00	10.37	7
ATOM	125	CA	ASN A	15	39.720	47.304	24.693	1.00	11.02	6	ATOM	178	CA	LYS A	21	26.731	48.544	24.164	1.00	11.61	6
ATOM	126	CB	ASN A	15	41.073	47.318	25.411	1.00	11.27	6	ATOM	179	CB	LYS A	21	27.348	49.856	23.671	1.00	15.11	6
ATOM	127	CG	ASN A	15	41.055	48.247	26.614	1.00	11.89	6	ATOM	180	CG	LYS A	21	27.086	50.981	24.674	1.00	21.25	6
ATOM	128	OO1	ASN A	15	40.008	48.358	27.277	1.00	12.57	8	ATOM	181	CO	LYS A	21	28.020	52.128	24.411	1.00	25.92	6
ATOM	129	WD2	ASN A	15	42.158	48.898	26.922	1.00	11.38	7	ATOM	182	CE	LYS A	21	27.600	53.426	25.067	1.00	30.86	6
ATOM	130	C	ASN A	15	39.240	48.737	24.377	1.00	11.05	6	ATOM	183	NZ	LYS A	21	27.119	54.448	24.030	1.00	34.41	7
ATOM	131	O	ASN A	15	39.932	49.767	24.524	1.00	11.08	8	ATOM	184	C	LYS A	21	26.551	47.632	22.934	1.00	11.59	6
ATOM	132	H	ASP A	16	38.008	48.835	23.905	1.00	10.98	7	ATOM	185	O	LYS A	21	25.474	47.562	22.400	1.00	11.80	8
ATOM	133	CA	ASP A	16	37.446	50.118	23.329	1.00	11.17	6	ATOM	186	N	ARG A	22	27.626	46.953	22.545	1.00	11.87	7
ATOM	134	CB	ASP A	16	36.924	50.059	22.068	1.00	11.99	6	ATOM	187	CA	ARG A	22	27.576	46.015	21.451	1.00	12.42	6
ATOM	135	CG	ASP A	16	35.761	49.101	21.873	1.00	12.89	6	ATOM	188	CG	ARG A	22	28.940	45.391	21.199	1.00	12.84	6
ATOM	136	OO1	ASP A	16	35.313	48.341	22.772	1.00	11.83	8	ATOM	189	CG	ARG A	22	29.804	46.215	20.240	1.00	13.26	6
ATOM	137	OO2	ASP A	16	35.244	49.114	20.732	1.00	14.31	8	ATOM	190	CO	ARG A	22	31.043	45.363	19.942	1.00	14.67	6
ATOM	138	C	ASP A	16	36.352	50.518	24.498	1.00	11.03	6	ATOM	191	HE	ARG A	22	32.084	45.253	20.955	1.00	14.04	7
ATOM	139	O	ASP A	16	35.768	51.582	24.289	1.00	11.12	8	ATOM	192	C2	ARG A	22	33.068	46.161	21.065	1.00	16.66	6
ATOM	140	H	GLY A	17	36.013	49.732	25.513	1.00	10.89	7	ATOM	193	WH1	ARG A	22	33.913	45.855	22.063	1.00	13.42	7
ATOM	141	CA	GLY A	17	34.972	50.083	26.479	1.00	10.61	6	ATOM	194	WH2	ARG A	22	33.206	47.242	20.261	1.00	12.34	7
ATOM	142	C	GLY A	17	33.545	50.032	25.938	1.00	10.65	6	ATOM	195	C	ARG A	22	26.586	44.921	21.812	1.00	12.77	6
ATOM	143	O	GLY A	17	32.629	50.522	26.601	1.00	10.67	8	ATOM	196	O	ARG A	22	25.682	44.543	21.038	1.00	13.11	8
ATOM	144	H	GLN A	18	33.287	49.436	24.766	1.00	10.50	7	ATOM	197	N	LEU A	23	26.678	44.342	23.002	1.00	12.84	7
ATOM	145	CA	GLN A	18	31.995	49.346	24.151	1.00	10.55	6	ATOM	198	CA	LEU A	23	25.698	43.292	23.370	1.00	12.86	6
ATOM	146	CB	GLN A	18	32.064	49.835	22.691	1.00	15.25	6	ATOM	199	CG	LEU A	23	26.092	42.716	24.721	1.00	10.68	6
ATOM	147	CG	GLN A	18	32.718	51.182	22.436	1.00	21.24	6	ATOM	200	CG	LEU A	23	25.126	41.739	25.361	1.00	10.16	6
ATOM	148	CO	GLN A	18	31.729	52.313	22.693	1.00	25.84	6	ATOM	201	CD1	LEU A	23	24.804	40.562	24.449	1.00	8.43	6
ATOM	149	OE1	GLN A	18	30.674	52.415	22.016	1.00	29.22	7	ATOM	202	CD2	LEU A	23	25.769	41.258	26.669	1.00	9.16	6
ATOM	150	ME2	GLN A	18	32.104	53.124	23.668	1.00	27.29	7	ATOM	203	C	LEU A	23	24.285	43.874	23.388	1.00	13.25	6
ATOM	151	C	GLN A	18	31.421	47.936	24.062	1.00	10.04	6	ATOM	204	O	LEU A	23	23.302	43.247	22.969	1.00	12.84	8
ATOM	152	O	GLN A	18	30.467	47.808	23.281	1.00	9.96	8	ATOM	205	N	GLN A	24	24.144	45.123	23.873	1.00	13.66	7
ATOM	153	H	HIS A	19	31.986	46.944	24.702	1.00	9.66	7	ATOM	206	CA	GLN A	24	22.848	45.781	23.929	1.00	14.44	6
ATOM	154	CA	HIS A	19	31.440	45.572	24.582	1.00	9.29	6	ATOM	207	CB	GLN A	24	22.959	47.205	24.523	1.00	16.30	6
ATOM	155	CB	HIS A	19	32.412	44.535	25.162	1.00	6.70	6	ATOM	208	CG	GLN A	24	21.578	47.851	24.620	1.00	18.17	6
ATOM	156	CG	HIS A	19	32.091	43.173	26.563	1.00	8.79	6	ATOM	209	CD	GLN A	24	21.659	49.208	25.296	1.00	20.30	6
ATOM	157	CD2	HIS A	19	31.749	41.987	25.138	1.00	7.93	6	ATOM	210	OE1	GLN A	24	22.651	49.936	25.205	1.00	20.53	7
ATOM	158	WD1	HIS A	19	32.116	42.955	23.187	1.00	8.36	7	ATOM	211	ME2	GLN A	24	20.619	49.539	26.023	1.00	20.53	7
ATOM	159	CE1	HIS A	19	31.825	41.705	22.909	1.00	8.32	6	ATOM	212	C	GLN A	24	22.208	45.914	22.528	1.00	14.70	6

ATOM	213	O	GLM	A	24	21.030	45.626	22.296	1.00	14.63	8
ATOM	214	N	ASN	A	25	23.034	46.369	21.594	1.00	14.90	7
ATOM	215	CA	ASN	A	25	22.642	46.325	20.213	1.00	15.31	6
ATOM	216	CB	ASN	A	25	23.645	47.256	19.304	1.00	18.01	6
ATOM	217	CG	ASN	A	25	23.711	48.719	19.680	1.00	22.28	6
ATOM	218	OO1	ASN	A	25	22.686	49.238	20.127	1.00	24.44	7
ATOM	219	MO2	ASN	A	25	24.836	49.432	19.588	1.00	23.11	8
ATOM	220	C	ASN	A	25	22.371	45.141	19.588	1.00	15.19	6
ATOM	221	O	ASN	A	25	21.542	45.198	18.637	1.00	15.31	8
ATOM	222	N	ASP	A	26	22.954	44.059	20.051	1.00	14.67	7
ATOM	223	CA	ASP	A	26	22.647	42.765	19.394	1.00	14.48	6
ATOM	224	CB	ASP	A	26	24.002	42.002	19.440	1.00	14.63	6
ATOM	225	CG	ASP	A	26	24.360	41.059	18.322	1.00	14.74	6
ATOM	226	OO1	ASP	A	26	23.651	41.073	17.292	1.00	14.77	8
ATOM	227	OO2	ASP	A	26	25.294	40.238	18.363	1.00	14.65	8
ATOM	228	C	ASP	A	26	21.497	41.933	19.949	1.00	14.18	6
ATOM	229	O	ASP	A	26	21.119	40.869	19.454	1.00	13.76	8
ATOM	230	N	ALA	A	27	20.813	42.356	20.986	1.00	14.32	7
ATOM	231	CA	ALA	A	27	19.761	41.641	21.661	1.00	14.78	6
ATOM	232	CB	ALA	A	27	19.276	42.463	22.849	1.00	12.97	6
ATOM	233	O	ALA	A	27	18.627	41.207	20.754	1.00	15.34	6
ATOM	234	O	ALA	A	27	18.231	40.028	20.840	1.00	15.36	8
ATOM	235	N	GLU	A	28	18.099	42.032	19.858	1.00	15.76	7
ATOM	236	CA	GLU	A	28	17.010	41.598	18.984	1.00	23.00	6
ATOM	237	CB	GLU	A	28	16.526	42.815	18.170	1.00	23.05	6
ATOM	238	CG	GLU	A	28	15.097	42.736	17.596	1.00	31.01	6
ATOM	239	CD	GLU	A	28	14.001	42.258	18.547	1.00	36.48	6
ATOM	240	OE1	GLU	A	28	13.644	41.013	18.587	1.00	40.16	8
ATOM	241	OE2	GLU	A	28	13.427	43.089	19.316	1.00	38.33	8
ATOM	242	C	GLU	A	28	17.410	40.467	18.044	1.00	15.55	6
ATOM	243	O	GLU	A	28	16.773	39.435	17.835	1.00	15.27	8
ATOM	244	N	HIS	A	29	18.577	40.712	17.415	1.00	15.36	7
ATOM	245	CA	HIS	A	29	19.158	39.769	16.461	1.00	15.11	6
ATOM	246	CB	HIS	A	29	20.492	40.422	16.008	1.00	16.22	6
ATOM	247	CG	HIS	A	29	21.296	39.400	15.259	1.00	18.29	6
ATOM	248	CD	HIS	A	29	20.895	38.501	14.294	1.00	18.16	6
ATOM	249	MO1	HIS	A	29	22.639	39.155	15.496	1.00	18.52	7
ATOM	250	CE1	HIS	A	29	23.055	38.163	14.693	1.00	18.61	6
ATOM	251	ME2	HIS	A	29	22.006	37.761	13.984	1.00	18.61	7
ATOM	252	C	HIS	A	29	19.282	38.370	17.059	1.00	14.84	6
ATOM	253	O	HIS	A	29	18.852	37.340	16.543	1.00	14.68	8
ATOM	254	N	LEU	A	30	19.913	38.292	18.233	1.00	14.66	7
ATOM	255	CA	LEU	A	30	20.154	37.107	19.020	1.00	14.56	6
ATOM	256	CB	LEU	A	30	20.913	37.409	20.319	1.00	13.60	6
ATOM	257	CG	LEU	A	30	22.350	37.884	20.194	1.00	15.00	6
ATOM	258	CD	LEU	A	30	23.018	37.967	21.586	1.00	15.90	6
ATOM	259	CO2	LEU	A	30	23.229	37.049	19.292	1.00	14.94	6
ATOM	260	C	LEU	A	30	18.833	36.434	19.390	1.00	14.68	6
ATOM	261	O	LEU	A	30	18.683	35.228	19.248	1.00	14.21	8
ATOM	262	N	SER	A	31	17.877	37.240	19.879	1.00	15.37	7
ATOM	263	CA	SER	A	31	16.596	36.559	20.204	1.00	16.15	6
ATOM	264	CB	SER	A	31	15.603	37.378	21.005	1.00	17.82	6
ATOM	265	CG	SER	A	31	15.358	38.528	20.190	1.00	22.98	8
ATOM	266	C	SER	A	31	15.995	36.112	18.852	1.00	16.34	6
ATOM	267	O	SER	A	31	15.558	34.966	18.878	1.00	16.30	8
ATOM	268	N	ASP	A	32	16.021	36.882	17.765	1.00	16.40	7
ATOM	269	CA	ASP	A	32	15.477	36.341	16.518	1.00	16.55	6
ATOM	270	CB	ASP	A	32	15.485	37.339	15.370	1.00	22.70	6
ATOM	271	CG	ASP	A	32	14.756	38.665	15.583	1.00	27.13	6
ATOM	272	OO1	ASP	A	32	13.849	38.871	16.443	1.00	29.59	8
ATOM	273	OO2	ASP	A	32	15.122	39.661	14.868	1.00	29.28	8
ATOM	274	C	ASP	A	32	16.207	35.103	16.032	1.00	16.39	6
ATOM	275	O	ASP	A	32	15.416	34.249	15.583	1.00	16.54	8
ATOM	276	N	ILE	A	33	17.519	34.862	16.111	1.00	15.83	7
ATOM	277	CA	ILE	A	33	18.093	33.612	15.639	1.00	15.16	6
ATOM	278	CB	ILE	A	33	19.570	33.804	15.292	1.00	13.80	6
ATOM	279	CG2	ILE	A	33	19.681	34.906	14.219	1.00	11.75	6
ATOM	280	CD1	ILE	A	33	20.353	34.167	16.549	1.00	13.86	6
ATOM	281	OO1	ILE	A	33	21.822	34.372	16.151	1.00	14.13	6
ATOM	282	C	ILE	A	33	17.939	32.408	16.568	1.00	15.00	6
ATOM	283	O	ILE	A	33	18.342	31.264	16.207	1.00	15.20	8
ATOM	284	N	GLY	A	34	17.303	32.527	17.740	1.00	14.35	7
ATOM	285	CA	GLY	A	34	17.113	31.380	18.606	1.00	13.52	6
ATOM	286	C	GLY	A	34	18.042	31.270	19.790	1.00	12.87	6
ATOM	287	O	GLY	A	34	18.034	30.216	20.453	1.00	12.97	8
ATOM	288	N	ILE	A	35	18.796	32.320	20.120	1.00	12.23	7
ATOM	289	CA	ILE	A	35	19.679	32.288	21.301	1.00	11.16	6
ATOM	290	CB	ILE	A	35	20.812	33.277	21.168	1.00	9.65	6
ATOM	291	CG2	ILE	A	35	21.595	33.376	22.527	1.00	8.10	6
ATOM	292	CG1	ILE	A	35	21.782	33.025	22.002	1.00	9.07	6
ATOM	293	CD1	ILE	A	35	22.447	31.654	19.909	1.00	8.99	6
ATOM	294	C	ILE	A	35	18.798	32.522	22.516	1.00	10.71	6
ATOM	295	O	ILE	A	35	18.050	33.521	22.584	1.00	10.65	8
ATOM	296	N	THR	A	36	18.816	31.638	23.519	1.00	10.23	7
ATOM	297	CA	THR	A	36	18.010	31.748	24.713	1.00	9.85	6
ATOM	298	CB	THR	A	36	17.144	30.482	24.943	1.00	7.65	6
ATOM	299	OG1	THR	A	36	18.091	29.405	25.089	1.00	7.88	8
ATOM	300	CG2	THR	A	36	16.198	30.293	23.779	1.00	6.33	6
ATOM	301	C	THR	A	36	18.844	32.120	25.955	1.00	9.79	6
ATOM	302	O	THR	A	36	18.271	32.449	26.995	1.00	9.82	8
ATOM	303	N	ALA	A	37	20.160	32.045	25.937	1.00	9.41	7
ATOM	304	CA	ALA	A	37	20.970	32.392	27.086	1.00	9.45	6
ATOM	305	CB	ALA	A	37	21.169	31.279	28.113	1.00	5.60	6
ATOM	306	C	ALA	A	37	22.309	32.897	26.536	1.00	9.43	6
ATOM	307	O	ALA	A	37	22.815	32.383	25.562	1.00	9.36	8
ATOM	308	N	VAL	A	38	22.871	33.921	27.171	1.00	9.63	7
ATOM	309	CA	VAL	A	38	24.164	34.496	26.851	1.00	9.68	6
ATOM	310	CB	VAL	A	38	24.047	35.995	26.455	1.00	12.81	6
ATOM	311	CG1	VAL	A	38	25.397	36.673	26.290	1.00	14.06	6
ATOM	312	CG2	VAL	A	38	23.287	36.191	25.123	1.00	12.91	6
ATOM	313	C	VAL	A	38	25.124	34.326	28.042	1.00	9.49	6
ATOM	314	O	VAL	A	38	24.720	34.563	29.197	1.00	9.06	7
ATOM	315	N	TRP	A	39	26.371	33.915	27.799	1.00	9.04	8
ATOM	316	CA	TRP	A	39	27.447	33.825	28.774	1.00	8.66	6
ATOM	317	CB	TRP	A	39	28.188	32.492	28.797	1.00	7.03	6
ATOM	318	CG	TRP	A	39	29.612	32.554	29.282	1.00	6.23	6

ATOM	319	CD2	TRP	A	39	30.691	31.682	28.807	1.00	6.00	6
ATOM	320	CE2	TRP	A	39	31.875	32.074	29.473	1.00	5.58	6
ATOM	321	CE3	TRP	A	39	30.708	30.585	27.908	1.00	5.00	6
ATOM	322	CD1	TRP	A	39	30.201	33.372	30.190	1.00	5.74	6
ATOM	323	WE1	TRP	A	39	31.568	33.153	30.268	1.00	5.57	6
ATOM	324	C22	TRP	A	39	33.099	31.441	29.211	1.00	5.00	6
ATOM	325	C23	TRP	A	39	31.955	29.964	27.701	1.00	5.00	6
ATOM	326	CH2	TRP	A	39	33.115	30.400	28.307	1.00	5.00	6
ATOM	327	C	TRP	A	39	28.317	35.078	28.452	1.00	8.53	6
ATOM	328	O	TRP	A	39	28.856	35.399	27.384	1.00	8.32	6
ATOM	329	N	ILE	A	40	28.431	35.945	29.459	1.00	8.37	7
ATOM	330	CA	ILE	A	40	29.143	37.247	29.467	1.00	8.51	6
ATOM	331	CB	ILE	A	40	28.091	38.113	30.259	1.00	9.85	6
ATOM	332	CG2	ILE	A	40	28.089	38.802	31.613	1.00	9.64	6
ATOM	333	CG1	ILE	A	40	27.803	39.287	29.286	1.00	9.52	6
ATOM	334	CD1	ILE	A	40	26.594	38.637	28.616	1.00	11.76	6
ATOM	335	C	ILE	A	40	30.524	37.121	30.043	1.00	8.39	6
ATOM	336	O	ILE	A	40	30.680	36.373	31.033	1.00	8.04	8
ATOM	337	N	PRO	A	41	31.571	37.800	29.564	1.00	8.30	7
ATOM	338	CO	PRO	A	41	31.469	38.773	28.451	1.00	8.06	6
ATOM	339	CA	PRO	A	41	32.887	37.771	30.151	1.00	8.14	6
ATOM	340	CB	PRO	A	41	33.802	38.683	29.246	1.00	8.13	6
ATOM	341	CG	PRO	A	41	32.756	39.565	28.595	1.00	8.01	6
ATOM	342	C	PRO	A	41	32.846	38.312	31.590	1.00	7.87	6
ATOM	343	O	PRO	A	41	31.891	38.952	32.039	1.00	7.72	8
ATOM	344	N	PRO	A	42	33.909	38.044	32.341	1.00	7.64	7
ATOM	345	CO	PRO	A	42	35.113	37.297	31.880	1.00	7.36	6
ATOM	346	CA	PRO	A	42	34.084	38.542	33.711	1.00	7.41	6
ATOM	347	CB	PRO	A	42	35.490	38.085	34.191	1.00	7.45	6
ATOM	348	CG	PRO	A	42	35.772	36.947	33.217	1.00	7.45	6
ATOM	349	C	PRO	A	42	33.841	40.054	33.685	1.00	7.06	6
ATOM	350	O	PRO	A	42	34.481	40.819	32.931	1.00	6.95	8
ATOM	351	N	ALA	A	43	32.875	40.536	34.452	1.00	6.53	7
ATOM	352	CA	ALA	A	43	32.477	41.937	34.681	1.00	6.39	6
ATOM	353	CB	ALA	A	43	30.968	41.991	34.756	1.00	5.00	6
ATOM	354	C	ALA	A	43	33.131	42.845	35.529	1.00	6.36	6
ATOM	355	O	ALA	A	43	32.847	44.042	35.582	1.00	6.42	8
ATOM	356	N	TYR	A	44	33.995	42.333	36.394	1.00	6.22	7
ATOM	357	CA	TYR	A	44	34.637	43.052	37.465	1.00	6.10	6
ATOM	358	CB	TYR	A	44	34.455	42.266	38.819	1.00	6.31	6
ATOM	359	CG	TYR	A	44	34.381	40.781	38.551	1.00	6.51	6
ATOM	360	CD1	TYR	A	44	35.538	40.086	38.145	1.00	6.67	6
ATOM	361	CE1	TYR	A	44	35.472	38.732	37.848	1.00	6.66	6
ATOM	362	CD2	TYR	A	44	33.200	40.071	38.613	1.00	6.52	6
ATOM	363	CE2	TYR	A	44	34.276	38.073	37.917	1.00	6.55	6
ATOM	364	C2	TYR	A	44	34.209	36.729	37.568	1.00	6.98	6
ATOM	365	OH	TYR	A	44	36.060	43.413	37.075	1.00	5.99	8
ATOM	366	C	TYR	A	44	36.060	43.413	37.075	1.00	5.98	8
ATOM	367	O	TYR	A	44	36.682	42.945	36.097	1.00	5.93	7
ATOM	368	N	LYS	A	45	36.556	44.410	37.815	1.00	5.73	6
ATOM	369	CA	LYS	A	45	37.865	45.003	37.587	1.00	5.00	6
ATOM	370	CB	LYS	A	45	38.033	44.160	38.580	1.00	5.00	6
ATOM	371	CG	LYS	A	45	39.192	47.127	38.251	1.00	5.00	6
ATOM	372	CD	LYS	A	45	39.093	48.021	37.024	1.00	5.00	6
ATOM	373	WE2	LYS	A	45	37.830	48.865	36.976	1.00	5.00	6
ATOM	374	CE	LYS	A	45	37.599	49.990	37.908	1.00	5.00	7
ATOM	375	C	LYS	A	45	39.029	44.010	37.657	1.00	5.87	6
ATOM	376	O	LYS	A	45	39.207	43.306	38.636	1.00	5.70	8
ATOM	377	N	GLY	A	46	39.847	43.978	36.608	1.00	6.09	7
ATOM	378	CA	GLY	A	46	41.017	43.149	36.478	1.00	6.70	6
ATOM	379	C	GLY	A	46	42.246	43.917	36.957	1.00	7.41	6
ATOM	380	O	GLY	A	46	42.171	45.098	37.382	1.00	7.54	8
ATOM	381	N	LEU	A	47	43.420	43.291	36.970	1.00	7.77	7
ATOM	382	CA	LEU	A	47	45.838	42.922	37.455	1.00	8.34	6
ATOM	383	CB	LEU	A	47	44.681	43.889	37.385	1.00	9.18	6
ATOM	384	CG	LEU	A	47	46.428	42.140	36.297	1.00	11.32	6
ATOM	385	CD1	LEU	A	47	45.419	41.207	35.660	1.00	12.40	6
ATOM	386	CD2	LEU	A	47	46.897	42.995	35.137	1.00	12.34	6
ATOM	387	C	LEU	A	47	45.040	45.105	36.483	1.00	8.70	6
ATOM	388	O	LEU	A	47	45.884	45.929	36.872	1.00	8.67	8
ATOM	389	N	SER	A	48	44.451	45.283	35.303	1.00	8.66	7
ATOM	390	CA	SER	A	48	46.667	46.453	34.457	1.00	9.11	6
ATOM	391	CB	SER	A	48	45.870	46.312	33.492	1.00	9.17	6
ATOM	392	CG	SER	A	48	45.546	45.387	32.490	1.00	8.88	8
ATOM	393	C	SER	A	48	43.380	46.678	33.672	1.00	9.13	6
ATOM	394	O	SER	A	48	42.533	45.777	33.610	1.00	9.05	8
ATOM	395	N	GLN	A	49	43.225	47.807	33.003	1.00	9.23	7
ATOM	396	CA	GLN	A	49	42.076	48.113	32.174	1.00	9.17	6
ATOM	397	CB	GLN	A	49	42.104	49.549	31.592	1.00	8.81	6
ATOM	398	CG	GLN	A	49	40.813	49.921	30.864	1.00	5.86	6
ATOM	399	CD	GLN	A	49	41.078	51.178	30.041	1.00	7.48	6
ATOM	400	OE1	GLN	A	49	41.898	51.153	29.103	1.00	7.62	8
ATOM	401	ME2	GLN	A	49	40.489	52.278	30.467	1.00	5.00	7
ATOM	402	C	GLN	A	49	41.929	47.121	31.006	1.00	9.30	6
ATOM	403	O	GLN	A	49	40.774	46.745	30.647	1.00	9.52	8
ATOM	404	N	SER	A	50	43.038	46.690	30.424	1.00	9.20	7
ATOM	405	CA	SER	A	50	42.992	45.763	29.281	1.00	9.33	6
ATOM	406	CB	SER	A	50	44.173	46.116	28.346	1.00	11.13	6
ATOM	407	CG	SER	A	50	45.417	45.891	29.000	1.00	14.96	8
ATOM	408	C	SER	A	50	42.924	44.272	29.626	1.00	8.88	6
ATOM	409	O	SER	A	50	42.810	43.409	28.736	1.00	8.96	8
ATOM	410	N	ASP	A	51	42.910	43.891	30.881	1.00	8.41	7
ATOM	411	CA	ASP	A	51	42.812	42.467	31.211	1.00	7.98	6
ATOM	412	CB	ASP	A	51	43.030	42.303	32.724	1.00	7.44	6
ATOM	413	CG	ASP	A	51	43.044	40.822	33.120	1.00	8.58	6
ATOM	414	CD1	ASP	A	51	44.069	40.115	32.869	1.00	8.63	8
ATOM	415	CD2	ASP	A	51	41.992	40.399	33.679	1.00	8.06	8
ATOM	416	C	ASP	A	51	41.460	41.932	30.766	1.00	7.80	6
ATOM	417	O	ASP	A	51	40.441	42.613	30.990	1.00	7.70	8
ATOM	418	N	ASN	A	52	41.330	40.729	30.217	1.00	7.56	7
ATOM	419	CA	ASN	A	52	40.040	40.182	29.867	1.00	7.47	6
ATOM	420	CB	ASN	A	52	40.175	38.887	29.057	1.00	9.45	6
ATOM	421	CG	ASN	A	52	40.562	39.187	27.620	1.00	12.85	8
ATOM	422	CD1	ASN	A	52	40.516	40.341	27.167	1.00	15.76	8
ATOM	423	MD2	ASN	A	52	40.979	38.239	26.786	1.00	12.70	7
ATOM	424	C	ASN	A	52	39.166	39.829	31.071	1.00	7.16	6

ATOM	425	O	ASN	A	52	38.007	39.399	30.782	1.00	7.11	8
ATOM	426	H	GLY	A	53	39.652	39.949	32.309	1.00	6.67	7
ATOM	427	CA	GLY	A	53	38.832	39.609	33.457	1.00	6.52	6
ATOM	428	C	GLY	A	53	39.262	38.324	34.124	1.00	6.62	6
ATOM	429	O	GLY	A	53	38.726	38.021	35.199	1.00	6.84	8
ATOM	430	N	TYR	A	54	40.227	37.565	33.548	1.00	6.28	7
ATOM	431	CA	TYR	A	54	40.722	36.331	34.179	1.00	5.98	6
ATOM	432	CB	TYR	A	54	41.027	35.227	33.116	1.00	6.06	6
ATOM	433	CG	TYR	A	54	39.720	34.834	32.427	1.00	5.99	6
ATOM	434	CD1	TYR	A	54	39.481	35.232	31.108	1.00	6.44	6
ATOM	435	CE1	TYR	A	54	38.251	34.920	30.492	1.00	6.68	6
ATOM	436	CE2	TYR	A	54	38.700	34.194	33.088	1.00	5.97	6
ATOM	437	CE2	TYR	A	54	37.474	33.857	32.517	1.00	6.05	6
ATOM	438	CZ	TYR	A	54	37.282	34.209	31.182	1.00	6.50	6
ATOM	439	OH	TYR	A	54	36.083	33.928	30.558	1.00	6.69	8
ATOM	440	O	TYR	A	54	42.441	35.655	35.818	1.00	5.63	8
ATOM	441	C	TYR	A	54	42.237	37.799	35.429	1.00	5.53	7
ATOM	442	H	GLY	A	55	43.226	38.205	36.438	1.00	5.64	6
ATOM	443	CA	GLY	A	55	42.464	39.315	37.256	1.00	5.59	6
ATOM	444	C	GLY	A	55	42.818	40.499	37.213	1.00	5.60	8
ATOM	445	O	GLY	A	55	41.410	38.876	37.948	1.00	5.20	7
ATOM	446	N	PRO	A	56	40.952	37.502	36.113	1.00	5.03	6
ATOM	447	CD	PRO	A	56	40.567	39.757	38.732	1.00	5.12	6
ATOM	448	CA	PRO	A	56	39.282	38.948	39.083	1.00	5.13	6
ATOM	449	CG	PRO	A	56	39.914	37.555	39.212	1.00	5.03	6
ATOM	450	CG	PRO	A	56	41.189	40.335	39.998	1.00	5.03	6
ATOM	451	C	PRO	A	56	41.728	39.671	40.862	1.00	5.00	8
ATOM	452	O	PRO	A	56	41.081	41.640	40.099	1.00	5.00	7
ATOM	453	N	TYR	A	57	41.499	42.474	41.207	1.00	5.00	6
ATOM	454	CA	TYR	A	57	42.042	43.842	40.709	1.00	5.45	6
ATOM	455	CB	TYR	A	57	42.261	44.833	41.840	1.00	6.29	6
ATOM	456	CG	TYR	A	57	43.330	44.634	42.730	1.00	6.84	6
ATOM	457	CD1	TYR	A	57	43.521	45.499	43.810	1.00	7.20	6
ATOM	458	CE1	TYR	A	57	41.421	45.913	42.014	1.00	6.52	6
ATOM	459	CE2	TYR	A	57	41.634	46.768	43.085	1.00	6.96	6
ATOM	460	CE2	TYR	A	57	42.835	47.431	45.036	1.00	7.37	6
ATOM	461	CZ	TYR	A	57	42.669	46.566	43.963	1.00	7.85	8
ATOM	462	OH	TYR	A	57	42.835	47.431	45.036	1.00	5.00	6
ATOM	463	C	TYR	A	57	40.546	42.347	43.362	1.00	5.00	6
ATOM	464	O	TYR	A	57	39.210	43.212	41.826	1.00	5.00	7
ATOM	465	N	ASP	A	58	38.134	43.465	42.771	1.00	5.00	6
ATOM	466	CA	ASP	A	58	38.136	44.990	43.088	1.00	5.00	6
ATOM	467	CB	ASP	A	58	37.210	45.478	44.152	1.00	5.00	6
ATOM	468	CG	ASP	A	58	36.550	44.681	44.829	1.00	5.00	8
ATOM	469	CD1	ASP	A	58	36.995	46.702	44.368	1.00	5.00	8
ATOM	470	CD2	ASP	A	58	36.813	42.974	42.250	1.00	5.00	6
ATOM	471	C	ASP	A	58	36.226	43.643	41.379	1.00	5.00	6
ATOM	472	O	ASP	A	58	34.967	41.399	42.426	1.00	5.00	6
ATOM	473	N	LEU	A	59	34.696	40.040	43.128	1.00	5.00	6
ATOM	474	CA	LEU	A	59	35.782	38.942	42.885	1.00	8.19	6
ATOM	475	CB	LEU	A	59	35.479	37.701	43.725	1.00	7.46	6
ATOM	476	CG	LEU	A	59						
ATOM	477	CD1	LEU	A	59						
ATOM	478	CD2	LEU	A	59						
ATOM	479	C	LEU	A	59						
ATOM	480	O	LEU	A	59						
ATOM	481	H	TYR	A	60						
ATOM	482	CA	TYR	A	60						
ATOM	483	CB	TYR	A	60						
ATOM	484	CG	TYR	A	60						
ATOM	485	CD1	TYR	A	60						
ATOM	486	CE1	TYR	A	60						
ATOM	487	CE2	TYR	A	60						
ATOM	488	CE2	TYR	A	60						
ATOM	489	OH	TYR	A	60						
ATOM	490	C	TYR	A	60						
ATOM	491	O	TYR	A	60						
ATOM	492	C	TYR	A	60						
ATOM	493	N	ASP	A	61						
ATOM	494	CA	ASP	A	61						
ATOM	495	CB	ASP	A	61						
ATOM	496	CG	ASP	A	61						
ATOM	497	CD1	ASP	A	61						
ATOM	498	CD2	ASP	A	61						
ATOM	499	C	ASP	A	61						
ATOM	500	O	ASP	A	61						
ATOM	501	H	LEU	A	62						
ATOM	502	CA	LEU	A	62						
ATOM	503	CB	LEU	A	62						
ATOM	504	CG	LEU	A	62						
ATOM	505	CD1	LEU	A	62						
ATOM	506	CD2	LEU	A	62						
ATOM	507	C	LEU	A	62						
ATOM	508	O	LEU	A	62						
ATOM	509	H	GLY	A	63						
ATOM	510	CA	GLY	A	63						
ATOM	511	C	GLY	A	63						
ATOM	512	O	GLY	A	63						
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ATOM	516	CG	GLU	A	64						
ATOM	517	CD	GLU	A	64						
ATOM	518	DE1	GLU	A	64						
ATOM	519	DE2	GLU	A	64						
ATOM	520	C	GLU	A	64						
ATOM	521	O	GLU	A	64						
ATOM	522	N	PHE	A	65						
ATOM	523	CA	PHE	A	65						
ATOM	524	CB	PHE	A	65						
ATOM	525	CG	PHE	A	65						
ATOM	526	CD1	PHE	A	65						
ATOM	527	CD2	PHE	A	65						
ATOM	528	CE1	PHE	A	65						
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ATOM	531	C	PHE A	65	36.480	53.123	40.126	1.00	10.75	6
ATOM	532	O	PHE A	65	36.935	52.381	39.255	1.00	10.67	8
ATOM	533	N	GLN A	66	37.091	54.215	40.584	1.00	11.02	7
ATOM	534	CA	GLN A	66	38.370	54.590	39.964	1.00	11.57	6
ATOM	535	CB	GLN A	66	38.512	56.102	40.168	1.00	15.18	6
ATOM	536	CG	GLN A	66	39.855	56.661	39.832	1.00	20.59	6
ATOM	537	CD	GLN A	66	40.150	56.793	38.363	1.00	20.59	6
ATOM	538	OE1	GLN A	66	39.958	57.812	37.688	1.00	28.38	8
ATOM	539	HE2	GLN A	66	40.716	55.789	37.719	1.00	28.38	7
ATOM	540	C	GLN A	66	39.489	53.768	40.576	1.00	11.54	6
ATOM	541	O	GLN A	67	39.989	54.089	41.699	1.00	11.29	8
ATOM	542	H	GLN A	67	39.870	52.683	39.895	1.00	11.31	7
ATOM	543	CA	GLN A	67	40.915	51.786	40.411	1.00	11.24	6
ATOM	544	CB	GLN A	67	40.390	50.591	42.242	1.00	9.56	6
ATOM	545	CG	GLN A	67	39.353	50.740	42.242	1.00	9.56	6
ATOM	546	CD	GLN A	67	38.970	49.695	43.240	1.00	6.97	6
ATOM	547	OE1	GLN A	67	39.359	49.865	44.405	1.00	7.23	8
ATOM	548	HE2	GLN A	67	38.222	48.659	42.932	1.00	5.00	7
ATOM	549	C	GLN A	67	41.738	51.246	39.242	1.00	11.63	6
ATOM	550	O	GLN A	67	41.158	50.867	38.216	1.00	11.46	8
ATOM	551	H	LYS A	68	43.063	51.149	39.341	1.00	12.10	6
ATOM	552	CA	LYS A	68	43.938	50.664	38.285	1.00	12.61	6
ATOM	553	CB	LYS A	68	43.621	49.280	37.709	1.00	13.06	6
ATOM	554	CG	LYS A	68	43.465	48.179	38.780	1.00	14.46	6
ATOM	555	CD	LYS A	68	44.715	48.024	39.626	1.00	15.01	6
ATOM	556	CE	LYS A	68	44.683	47.225	40.918	1.00	14.26	6
ATOM	557	NZ	LYS A	68	46.062	47.066	41.699	1.00	12.89	7
ATOM	558	O	LYS A	68	43.908	51.710	37.178	1.00	13.39	6
ATOM	559	H	GLY A	69	43.978	51.422	35.955	1.00	14.41	8
ATOM	560	N	GLY A	69	43.764	53.001	37.484	1.00	13.13	7
ATOM	561	CA	GLY A	69	43.739	54.115	36.582	1.00	12.76	6
ATOM	562	C	GLY A	69	42.535	54.177	35.674	1.00	12.59	6
ATOM	563	O	GLY A	69	42.481	54.975	34.735	1.00	12.74	8
ATOM	564	N	THR A	70	41.497	53.394	35.983	1.00	12.05	7
ATOM	565	CA	THR A	70	40.325	53.375	35.120	1.00	11.09	6
ATOM	566	CB	THR A	70	40.536	52.215	34.122	1.00	9.79	6
ATOM	567	CG2	THR A	70	39.502	52.210	33.117	1.00	10.12	8
ATOM	568	CD	THR A	70	40.547	50.831	34.773	1.00	9.26	6
ATOM	569	C	THR A	70	39.087	53.169	35.950	1.00	10.63	6
ATOM	570	O	THR A	71	39.115	52.524	36.977	1.00	10.42	8
ATOM	571	N	VAL A	71	37.978	53.737	35.484	1.00	10.18	7
ATOM	572	CA	VAL A	71	36.690	53.549	36.107	1.00	9.77	6
ATOM	573	CB	VAL A	71	35.802	54.788	35.985	1.00	10.20	6
ATOM	574	CG1	VAL A	71	34.374	54.448	36.303	1.00	8.33	6
ATOM	575	CG2	VAL A	71	36.393	55.860	36.919	1.00	9.35	6
ATOM	576	C	VAL A	71	36.093	52.313	35.404	1.00	9.37	6
ATOM	577	O	VAL A	71	35.766	51.299	36.050	1.00	9.39	8
ATOM	578	N	ARG A	72	36.007	52.357	36.089	1.00	8.79	7
ATOM	579	CA	ARG A	72	35.449	51.252	33.344	1.00	8.64	6
ATOM	580	CB	ARG A	72	35.205	51.645	31.846	1.00	7.09	6
ATOM	581	CG	ARG A	72	36.443	51.798	30.962	1.00	6.38	6
ATOM	582	CD	ARG A	72	36.054	51.979	29.499	1.00	6.64	6
ATOM	583	HE	ARG A	72	37.131	52.071	28.536	1.00	6.31	7
ATOM	584	CZ	ARG A	72	38.053	51.266	28.054	1.00	5.00	6
ATOM	585	NH1	ARG A	72	38.926	51.664	27.158	1.00	5.00	7
ATOM	586	NH2	ARG A	72	38.043	50.022	28.506	1.00	5.00	7
ATOM	587	C	ARG A	72	36.316	49.984	33.347	1.00	8.29	6
ATOM	588	O	ARG A	72	37.531	50.080	33.499	1.00	8.41	8
ATOM	589	N	THR A	73	35.700	48.836	33.120	1.00	8.00	7
ATOM	590	CA	THR A	73	36.539	47.632	32.967	1.00	8.12	6
ATOM	591	CB	THR A	73	35.820	46.301	33.270	1.00	6.10	6
ATOM	592	CG1	THR A	73	34.727	46.140	32.317	1.00	5.35	8
ATOM	593	CG2	THR A	73	35.361	46.223	34.730	1.00	5.00	6
ATOM	594	C	THR A	73	36.932	47.628	31.481	1.00	8.12	6
ATOM	595	O	THR A	73	36.630	48.581	30.739	1.00	8.16	8
ATOM	596	N	LYS A	74	37.514	46.575	30.939	1.00	8.08	7
ATOM	597	CA	LYS A	74	37.782	46.496	29.508	1.00	8.07	6
ATOM	598	CB	LYS A	74	38.443	45.122	29.215	1.00	7.57	6
ATOM	599	CG	LYS A	74	38.780	44.864	27.777	1.00	7.31	6
ATOM	600	CD	LYS A	74	39.173	43.465	27.359	1.00	6.71	6
ATOM	601	CE	LYS A	74	39.463	43.461	25.867	1.00	7.86	6
ATOM	602	NZ	LYS A	74	40.043	42.121	25.465	1.00	7.32	7
ATOM	603	C	LYS A	74	36.469	46.596	28.696	1.00	7.96	6
ATOM	604	O	LYS A	74	36.376	47.163	27.598	1.00	7.92	8
ATOM	605	N	THR A	75	35.375	46.004	29.221	1.00	7.80	7
ATOM	606	CA	THR A	75	34.113	45.937	28.503	1.00	7.58	6
ATOM	607	CB	THR A	75	34.311	43.409	28.864	1.00	7.14	6
ATOM	608	CG	THR A	75	34.853	42.777	29.988	1.00	6.37	6
ATOM	609	CD1	THR A	75	35.716	41.696	29.857	1.00	6.28	6
ATOM	610	CE1	THR A	75	34.677	42.916	27.589	1.00	6.45	6
ATOM	611	CD2	THR A	75	35.547	41.855	27.414	1.00	6.14	6
ATOM	612	CE2	THR A	75	36.039	41.257	28.570	1.00	6.23	8
ATOM	613	C	THR A	75	36.913	40.195	28.479	1.00	6.33	8
ATOM	614	OH	THR A	75	33.188	47.141	28.576	1.00	7.81	6
ATOM	615	O	THR A	75	32.274	47.302	27.713	1.00	7.79	8
ATOM	616	N	GLY A	76	33.355	48.068	29.555	1.00	7.71	7
ATOM	617	CA	GLY A	76	32.468	49.243	29.681	1.00	7.27	6
ATOM	618	C	GLY A	76	32.204	49.486	31.152	1.00	7.13	6
ATOM	619	O	GLY A	76	32.841	48.904	32.048	1.00	6.91	8
ATOM	620	N	THR A	77	31.250	50.356	31.425	1.00	7.24	7
ATOM	621	CA	THR A	77	30.855	50.694	32.813	1.00	7.52	6
ATOM	622	CB	THR A	77	30.366	52.172	32.914	1.00	7.84	6
ATOM	623	CG	THR A	77	29.223	52.337	32.073	1.00	8.21	8
ATOM	624	CG1	THR A	77	31.378	53.173	32.361	1.00	6.70	6
ATOM	625	CG2	THR A	77	29.712	49.827	33.304	1.00	7.62	6
ATOM	626	C	THR A	77	28.984	49.118	32.575	1.00	7.39	8
ATOM	627	O	THR A	77	29.460	49.853	34.611	1.00	7.89	7
ATOM	628	N	LYS A	78	28.398	49.084	35.247	1.00	8.24	6
ATOM	629	CA	LYS A	78	28.465	49.384	36.759	1.00	8.57	6
ATOM	630	CB	LYS A	78	27.449	48.604	37.551	1.00	11.52	6
ATOM	631	CG	LYS A	78	27.592	49.117	39.004	1.00	13.82	6
ATOM	632	CD	LYS A	78	26.681	48.228	39.824	1.00	15.45	6
ATOM	633	CE	LYS A	78	26.132	49.000	40.954	1.00	18.28	7
ATOM	634	NZ	LYS A	78	27.022	49.428	34.735	1.00	8.73	6
ATOM	635	C	LYS A	78	26.165	48.565	34.477	1.00	8.67	8
ATOM	636	O	LYS A	78						

ATOM	637	N	SER	A	79	26.749	50.759	34.578	1.00	9.32	7	19.100	44.530	30.757	1.00	11.09	7
ATOM	638	CA	SER	A	79	25.401	51.141	34.086	1.00	9.71	6	17.669	44.837	30.621	1.00	11.74	6
ATOM	639	CB	SER	A	79	25.190	52.607	34.380	1.00	12.14	6	17.181	44.628	29.181	1.00	12.11	6
ATOM	640	OG	SER	A	79	25.960	53.338	33.488	1.00	15.84	8	16.109	44.068	28.922	1.00	12.28	8
ATOM	641	C	SER	A	79	25.262	50.703	32.644	1.00	9.79	6	17.881	45.069	28.130	1.00	12.31	7
ATOM	642	O	SER	A	79	24.142	50.254	32.312	1.00	10.15	8	17.451	44.776	26.770	1.00	12.79	6
ATOM	643	N	GLU	A	80	26.291	50.128	31.816	1.00	9.56	7	18.466	45.329	25.735	1.00	13.98	6
ATOM	644	CA	GLU	A	80	26.160	50.655	30.452	1.00	9.39	6	18.420	46.745	26.044	1.00	18.72	8
ATOM	645	CB	GLU	A	80	27.429	50.452	29.723	1.00	10.04	6	17.310	43.266	26.465	1.00	12.80	6
ATOM	646	CG	GLU	A	80	27.546	51.928	29.378	1.00	11.54	6	16.395	42.812	25.776	1.00	12.92	8
ATOM	647	OG	GLU	A	80	28.902	52.167	28.769	1.00	14.36	6	18.262	42.459	26.958	1.00	12.48	7
ATOM	648	OE1	GLU	A	80	29.881	51.408	28.913	1.00	15.28	8	18.199	41.020	26.764	1.00	12.30	6
ATOM	649	OE2	GLU	A	80	29.051	53.186	28.075	1.00	18.22	8	20.738	40.582	27.265	1.00	10.21	6
ATOM	650	C	GLU	A	80	25.853	48.629	30.476	1.00	9.05	6	21.896	40.339	27.265	1.00	10.80	6
ATOM	651	O	GLU	A	80	25.005	48.179	29.720	1.00	8.72	8	20.566	39.947	25.036	1.00	11.89	6
ATOM	652	N	LEU	A	81	26.441	47.873	31.394	1.00	9.09	7	16.594	39.915	31.863	1.00	11.47	6
ATOM	653	CA	LEU	A	81	26.145	46.428	31.534	1.00	9.12	6	17.072	38.635	31.719	1.00	11.34	6
ATOM	654	CB	LEU	A	81	27.188	45.716	32.385	1.00	8.24	6	16.258	39.375	26.993	1.00	12.29	8
ATOM	655	CG	LEU	A	81	26.866	44.272	32.883	1.00	8.68	6	16.784	40.866	28.752	1.00	12.11	7
ATOM	656	CD1	LEU	A	81	26.744	43.229	31.731	1.00	7.74	6	15.679	40.323	29.507	1.00	12.49	6
ATOM	657	CD2	LEU	A	81	27.983	43.841	33.771	1.00	9.60	6	15.713	40.745	30.987	1.00	11.47	6
ATOM	658	C	LEU	A	81	24.710	46.226	32.053	1.00	9.19	6	16.594	39.915	31.863	1.00	11.05	6
ATOM	659	O	LEU	A	81	23.952	45.386	31.515	1.00	8.94	8	17.117	40.353	33.037	1.00	10.31	7
ATOM	660	N	GLN	A	82	24.247	47.005	33.042	1.00	9.81	7	17.837	38.363	32.823	1.00	11.68	7
ATOM	661	CA	GLN	A	82	22.853	46.834	33.479	1.00	9.33	6	17.865	39.425	33.593	1.00	10.84	6
ATOM	662	CB	GLN	A	82	22.588	47.739	34.681	1.00	11.55	6	14.378	40.741	28.838	1.00	13.05	6
ATOM	663	CG	GLN	A	82	23.288	47.105	33.901	1.00	14.03	6	13.480	39.910	28.764	1.00	12.72	8
ATOM	664	CD	GLN	A	82	23.239	47.993	37.132	1.00	10.46	6	14.275	41.957	28.285	1.00	13.89	7
ATOM	665	OE1	GLN	A	82	23.497	49.180	36.990	1.00	15.76	8	12.957	42.281	27.665	1.00	15.19	6
ATOM	666	NE2	GLN	A	82	22.947	47.380	38.266	1.00	10.18	7	12.784	43.796	27.578	1.00	14.96	6
ATOM	667	C	GLN	A	82	21.878	47.108	32.358	1.00	10.17	6	12.761	44.225	26.638	1.00	19.72	8
ATOM	668	O	GLN	A	82	20.854	46.455	32.247	1.00	10.30	8	12.722	41.472	26.411	1.00	15.94	6
ATOM	669	N	ASP	A	83	22.106	48.088	31.501	1.00	10.58	7	11.612	41.428	25.924	1.00	15.88	8
ATOM	670	CA	ASP	A	83	21.281	48.355	30.317	1.00	11.05	6	13.632	40.675	25.854	1.00	16.85	7
ATOM	671	CB	ASP	A	83	21.631	49.619	29.516	1.00	15.09	6	13.529	39.799	24.719	1.00	17.41	6
ATOM	672	CG	ASP	A	83	21.228	50.893	30.246	1.00	18.79	6	14.651	39.930	23.689	1.00	20.09	6
ATOM	673	CD1	ASP	A	83	20.404	50.950	31.175	1.00	18.59	8	14.977	41.395	23.474	1.00	23.93	6
ATOM	674	CD2	ASP	A	83	21.832	51.914	29.841	1.00	22.13	8	14.271	41.859	22.236	1.00	27.09	6
ATOM	675	C	ASP	A	83	21.439	47.203	29.307	1.00	10.81	6	14.479	43.230	22.020	1.00	31.65	7
ATOM	676	O	ASP	A	83	20.391	46.942	28.751	1.00	11.02	8	15.007	44.382	22.298	1.00	33.62	6
ATOM	677	N	ALA	A	84	22.562	46.574	29.048	1.00	10.37	7	15.835	44.587	23.321	1.00	33.94	7
ATOM	678	CA	ALA	A	84	22.630	45.461	28.120	1.00	10.32	6	16.682	45.428	21.512	1.00	34.30	7
ATOM	679	CB	ALA	A	84	24.057	45.019	27.847	1.00	7.64	6	13.594	38.341	25.184	1.00	17.75	6
ATOM	680	C	ALA	A	84	21.758	44.332	28.688	1.00	10.46	6	13.827	37.473	24.356	1.00	17.92	8
ATOM	681	O	ALA	A	84	20.988	43.692	27.919	1.00	10.32	8	13.635	38.126	26.487	1.00	17.94	7
ATOM	682	N	ILE	A	85	21.828	44.045	29.995	1.00	10.47	7	13.471	36.780	27.044	1.00	17.98	6
ATOM	683	CA	ILE	A	85	21.036	42.985	30.642	1.00	10.46	6	12.229	35.993	26.546	1.00	26.48	6
ATOM	684	CB	ILE	A	85	21.501	42.710	32.116	1.00	9.71	6	11.010	36.657	27.191	1.00	29.10	6
ATOM	685	CG2	ILE	A	85	20.474	41.875	32.906	1.00	6.40	6	10.782	36.615	28.414	1.00	31.71	8
ATOM	686	OG1	ILE	A	85	22.921	42.132	32.080	1.00	9.01	6	10.235	37.344	26.343	1.00	30.92	7
ATOM	687	CD1	ILE	A	85	23.684	42.092	33.399	1.00	10.12	6	14.740	35.989	26.780	1.00	17.40	6
ATOM	688	C	ILE	A	85	19.543	43.282	30.566	1.00	10.65	6	14.762	34.799	26.423	1.00	17.64	8
ATOM	689	O	ILE	A	85	18.768	42.340	30.313	1.00	10.41	8						

ATOM	743	H	VAL	A	93	15.886	36.642	26.989	1.00	16.55	7	796	O	VAL	A	99	36.461	31.987	37.850	1.00	6.46	8
ATOM	744	CA	VAL	A	93	17.213	36.038	26.833	1.00	15.28	6	797	N	VAL	A	100	35.082	34.017	38.489	1.00	6.60	7
ATOM	745	CB	VAL	A	93	18.120	36.688	25.785	1.00	12.97	6	798	CA	VAL	A	100	36.487	33.766	38.594	1.00	6.45	6
ATOM	746	CG1	VAL	A	93	19.467	36.021	25.989	1.00	11.55	6	799	CB	VAL	A	100	37.273	34.786	37.735	1.00	6.89	6
ATOM	747	CG2	VAL	A	93	17.378	36.751	24.553	1.00	12.58	6	800	CG1	VAL	A	100	38.728	34.308	37.697	1.00	6.74	6
ATOM	748	C	VAL	A	93	17.771	36.161	28.256	1.00	14.60	6	801	CG2	VAL	A	100	36.761	34.893	36.314	1.00	6.94	6
ATOM	749	O	VAL	A	93	17.736	37.228	28.829	1.00	14.36	8	802	C	VAL	A	100	36.930	33.803	40.041	1.00	6.61	6
ATOM	750	N	GLN	A	94	18.211	35.007	28.742	1.00	13.97	7	803	O	VAL	A	100	37.306	34.866	40.566	1.00	6.72	7
ATOM	751	CA	GLN	A	94	18.792	34.812	30.045	1.00	13.10	6	804	N	LEU	A	101	36.882	32.651	40.724	1.00	6.41	7
ATOM	752	CB	GLN	A	94	18.642	33.375	30.542	1.00	13.62	6	805	CA	LEU	A	101	37.189	32.537	42.133	1.00	6.10	6
ATOM	753	CG	GLN	A	94	17.165	33.203	30.919	1.00	16.17	6	806	CB	LEU	A	101	36.017	31.716	42.731	1.00	7.20	6
ATOM	754	CD	GLM	A	94	17.047	31.828	31.552	1.00	19.51	6	807	CD	LEU	A	101	34.663	32.479	42.645	1.00	8.90	6
ATOM	755	OE1	GLM	A	94	17.710	30.855	31.198	1.00	21.76	8	808	OE1	LEU	A	101	33.657	31.509	43.300	1.00	9.60	6
ATOM	756	HE2	GLM	A	94	16.206	31.683	32.559	1.00	21.21	7	809	HE2	LEU	A	101	34.726	33.873	43.244	1.00	7.63	6
ATOM	757	C	GLN	A	94	20.275	35.223	30.003	1.00	12.28	6	810	C	LEU	A	101	38.456	31.843	42.579	1.00	5.96	6
ATOM	758	O	GLN	A	94	20.882	35.311	28.935	1.00	12.02	8	811	O	LEU	A	101	38.672	31.740	43.782	1.00	6.02	8
ATOM	759	N	VAL	A	95	20.772	35.576	31.218	1.00	11.32	7	812	N	ASN	A	102	39.260	31.326	41.676	1.00	5.73	7
ATOM	760	CA	VAL	A	95	22.144	36.030	31.272	1.00	10.46	6	813	CA	ASN	A	102	40.471	30.629	42.025	1.00	5.58	6
ATOM	761	CG1	VAL	A	95	22.215	37.553	31.568	1.00	11.92	6	814	CG	ASN	A	102	40.963	29.889	40.727	1.00	5.00	6
ATOM	762	CG1	VAL	A	95	23.646	38.014	31.735	1.00	12.03	6	815	CG	ASN	A	102	42.327	29.247	40.912	1.00	5.00	6
ATOM	763	CG2	VAL	A	95	21.591	38.367	30.411	1.00	12.21	6	816	CG1	ASN	A	102	42.309	28.218	41.608	1.00	5.00	8
ATOM	764	C	VAL	A	95	22.942	35.249	32.302	1.00	9.75	6	817	MD2	ASN	A	102	43.493	29.633	40.442	1.00	5.00	7
ATOM	765	O	VAL	A	95	22.559	35.259	33.483	1.00	9.63	8	818	O	ASN	A	102	41.580	31.490	42.620	1.00	5.69	6
ATOM	766	H	TYR	A	96	24.034	34.613	31.857	1.00	8.90	7	819	O	ASN	A	102	42.261	31.045	43.593	1.00	6.11	8
ATOM	767	CA	TYR	A	96	24.920	33.882	32.786	1.00	8.34	6	820	N	HIS	A	103	41.853	32.670	42.103	1.00	5.60	7
ATOM	768	CB	TYR	A	96	25.217	32.512	32.267	1.00	8.31	6	821	CA	HIS	A	103	42.935	33.520	42.506	1.00	5.59	6
ATOM	769	CG	TYR	A	96	24.055	31.583	31.987	1.00	8.37	6	822	CB	HIS	A	103	44.089	33.287	41.487	1.00	6.54	6
ATOM	770	CD1	TYR	A	96	24.298	30.500	31.130	1.00	8.46	6	823	CG	HIS	A	103	43.645	33.442	40.043	1.00	7.70	6
ATOM	771	CE1	TYR	A	96	23.255	29.643	30.831	1.00	8.30	6	824	CD2	HIS	A	103	43.560	34.512	39.230	1.00	6.52	6
ATOM	772	CD2	TYR	A	96	22.797	31.752	32.491	1.00	8.19	6	825	MD1	HIS	A	103	43.187	32.341	39.282	1.00	9.01	7
ATOM	773	CE2	TYR	A	96	21.762	30.928	32.186	1.00	8.05	6	826	CE1	HIS	A	103	42.794	32.769	38.082	1.00	8.40	6
ATOM	774	CZ	TYR	A	96	22.011	29.854	31.363	1.00	7.94	6	827	ME2	HIS	A	103	42.993	34.113	38.070	1.00	8.31	7
ATOM	775	OH	TYR	A	96	21.055	28.940	31.084	1.00	7.64	8	828	O	HIS	A	103	42.555	34.977	42.419	1.00	5.57	6
ATOM	776	C	TYR	A	96	26.218	34.655	33.000	1.00	8.00	6	829	O	HIS	A	103	41.470	35.229	41.899	1.00	5.20	8
ATOM	777	O	TYR	A	96	26.855	35.017	32.005	1.00	7.99	8	830	N	LYS	A	104	43.438	35.861	42.914	1.00	5.83	7
ATOM	778	N	GLY	A	97	26.624	34.919	34.243	1.00	7.85	7	831	CA	LYS	A	104	43.226	37.313	42.871	1.00	6.01	6
ATOM	779	CA	GLY	A	97	27.818	35.671	34.578	1.00	7.64	6	832	CB	LYS	A	104	42.938	37.971	44.213	1.00	8.00	6
ATOM	780	C	GLY	A	97	29.038	34.754	34.756	1.00	7.84	6	833	CG	LYS	A	104	41.748	37.393	44.978	1.00	8.52	6
ATOM	781	O	GLY	A	97	30.194	33.655	35.307	1.00	7.51	8	834	CD	LYS	A	104	41.373	38.324	46.133	1.00	9.80	6
ATOM	782	N	ASP	A	98	31.455	35.231	34.285	1.00	7.87	7	835	CE	LYS	A	104	40.973	39.748	45.746	1.00	8.97	6
ATOM	783	CA	ASP	A	98	31.555	34.409	34.482	1.00	8.04	6	836	NZ	LYS	A	104	39.514	39.723	45.383	1.00	8.50	7
ATOM	784	CB	ASP	A	98	32.546	34.944	33.523	1.00	7.77	6	837	O	LYS	A	104	44.489	37.894	42.278	1.00	6.11	6
ATOM	785	CG	ASP	A	98	33.452	33.828	33.077	1.00	7.80	6	838	C	LYS	A	104	45.526	37.321	42.649	1.00	6.50	8
ATOM	786	OO1	ASP	A	98	33.791	33.741	33.896	1.00	8.28	8	839	N	ALA	A	105	44.501	38.896	41.451	1.00	5.96	7
ATOM	787	OO2	ASP	A	98	33.919	33.761	31.896	1.00	8.14	8	840	CA	ALA	A	105	45.699	39.429	40.846	1.00	5.18	6
ATOM	788	C	ASP	A	98	31.868	34.688	35.953	1.00	7.80	6	841	CB	ALA	A	105	45.660	39.063	39.361	1.00	5.88	6
ATOM	789	O	ASP	A	98	31.644	35.739	36.518	1.00	7.83	8	842	C	ALA	A	105	45.785	40.943	41.031	1.00	6.37	6
ATOM	790	N	VAL	A	99	32.333	33.601	36.602	1.00	7.67	7	843	O	ALA	A	105	44.741	41.578	41.199	1.00	6.24	8
ATOM	791	CA	VAL	A	99	32.708	33.576	38.035	1.00	7.25	6	844	N	GLY	A	106	46.958	41.584	41.044	1.00	6.40	7
ATOM	792	CB	VAL	A	99	31.742	32.652	38.791	1.00	8.70	6	845	CA	GLY	A	106	47.040	43.001	41.190	1.00	6.60	6
ATOM	793	CG1	VAL	A	99	32.193	32.306	40.195	1.00	9.79	6	846	C	GLY	A	106	47.006	43.611	42.373	1.00	7.01	6
ATOM	794	CG2	VAL	A	99	30.366	33.362	38.885	1.00	9.90	6	847	O	GLY	A	106	46.524	44.736	42.659	1.00	6.76	8
ATOM	795	C	VAL	A	99	34.155	33.123	38.148	1.00	6.81	6	848	N	ALA	A	107	47.489	42.945	43.637	1.00	7.49	7

ATOM	849	CA	ALA	A 107	47.462	43.434	44.979	1.00	7.87	6	ATOM	902	C	THR	A 114	56.563	31.547	54.495	1.00	11.69	6
ATOM	850	CB	ALA	A 107	48.271	42.572	45.920	1.00	5.59	6	ATOM	903	O	THR	A 114	55.355	31.265	54.457	1.00	11.32	8
ATOM	851	C	ALA	A 107	48.055	44.842	44.970	1.00	8.71	6	ATOM	904	N	ALA	A 115	57.429	31.042	53.643	1.00	11.64	7
ATOM	852	O	ALA	A 107	48.875	45.204	44.120	1.00	8.95	8	ATOM	905	CA	ALA	A 115	57.024	30.048	52.638	1.00	11.55	6
ATOM	853	N	ASP	A 108	47.647	45.649	45.934	1.00	9.17	7	ATOM	906	CB	ALA	A 115	56.825	30.894	51.357	1.00	10.80	6
ATOM	854	CA	ASP	A 108	48.106	47.011	46.130	1.00	9.77	6	ATOM	907	C	ALA	A 115	58.039	28.947	52.343	1.00	11.45	6
ATOM	855	CB	ASP	A 108	47.118	47.666	47.155	1.00	10.59	6	ATOM	908	O	ALA	A 115	59.215	29.073	52.688	1.00	11.41	8
ATOM	856	CG	ASP	A 108	45.718	47.703	46.582	1.00	10.42	6	ATOM	909	N	VAL	A 116	57.641	27.868	51.657	1.00	11.33	7
ATOM	857	CO1	ASP	A 108	44.685	47.094	46.851	1.00	10.41	8	ATOM	910	CA	VAL	A 116	58.513	26.814	51.184	1.00	11.10	6
ATOM	858	CO2	ASP	A 108	45.580	48.455	45.604	1.00	12.47	8	ATOM	911	CB	VAL	A 116	58.338	25.436	51.815	1.00	12.23	6
ATOM	859	C	ASP	A 108	49.530	47.044	46.683	1.00	10.18	6	ATOM	912	CO1	VAL	A 116	58.978	25.449	53.208	1.00	12.01	6
ATOM	860	O	ASP	A 109	50.281	48.011	46.478	1.00	10.34	8	ATOM	913	CO2	VAL	A 116	56.802	26.978	51.873	1.00	11.15	6
ATOM	861	N	ALA	A 109	49.958	46.023	47.436	1.00	10.17	7	ATOM	914	C	VAL	A 116	58.250	26.642	49.656	1.00	10.95	6
ATOM	862	CA	ALA	A 109	51.273	45.970	48.023	1.00	10.21	6	ATOM	915	O	VAL	A 116	57.100	26.960	49.240	1.00	11.03	8
ATOM	863	CB	ALA	A 109	51.271	46.787	49.322	1.00	10.14	6	ATOM	916	N	GLU	A 117	59.187	26.205	48.856	1.00	10.29	7
ATOM	864	C	ALA	A 109	51.659	44.553	48.398	1.00	10.56	6	ATOM	917	CA	GLU	A 117	58.932	25.898	47.465	1.00	10.06	6
ATOM	865	O	ALA	A 109	50.836	43.629	48.473	1.00	10.49	8	ATOM	918	CB	GLU	A 117	60.201	25.861	46.625	1.00	11.90	6
ATOM	866	CA	THR	A 110	52.966	44.438	48.710	1.00	10.14	7	ATOM	919	CG	GLU	A 117	60.905	27.201	46.773	1.00	14.30	6
ATOM	867	CB	THR	A 110	53.504	43.168	49.132	1.00	11.01	6	ATOM	920	CD	GLU	A 117	62.245	27.143	46.070	1.00	16.13	6
ATOM	868	CB	THR	A 110	54.958	42.954	48.705	1.00	11.26	6	ATOM	921	OE1	GLU	A 117	62.515	28.342	45.175	1.00	16.80	8
ATOM	869	OG1	THR	A 110	55.741	43.988	49.294	1.00	11.23	6	ATOM	922	OE2	GLU	A 117	63.067	28.004	46.366	1.00	17.32	8
ATOM	870	CG2	THR	A 110	55.196	43.055	47.209	1.00	11.79	8	ATOM	923	C	GLU	A 117	58.354	24.480	47.369	1.00	9.47	8
ATOM	871	C	THR	A 110	53.445	43.091	50.643	1.00	11.37	6	ATOM	924	O	GLU	A 117	58.596	23.656	48.258	1.00	9.47	8
ATOM	872	O	THR	A 110	53.349	44.102	51.351	1.00	11.33	8	ATOM	925	N	VAL	A 118	57.623	26.157	46.316	1.00	9.40	7
ATOM	873	N	GLU	A 111	53.477	41.851	51.165	1.00	11.70	7	ATOM	926	CA	VAL	A 118	56.987	22.802	46.152	1.00	9.25	6
ATOM	874	CA	GLU	A 111	53.527	41.504	52.566	1.00	11.89	6	ATOM	927	CB	VAL	A 118	55.556	23.243	46.543	1.00	10.55	6
ATOM	875	CB	GLU	A 111	52.223	40.870	53.035	1.00	10.98	6	ATOM	928	CG1	VAL	A 118	54.529	23.164	45.421	1.00	9.52	6
ATOM	876	CG	GLU	A 111	51.153	41.995	53.103	1.00	13.17	6	ATOM	929	CG2	VAL	A 118	55.061	22.664	47.855	1.00	10.49	6
ATOM	877	CD	GLU	A 111	49.812	41.428	53.483	1.00	14.55	6	ATOM	930	C	VAL	A 118	57.360	22.305	44.765	1.00	9.31	6
ATOM	878	OE1	GLU	A 111	49.365	40.456	52.823	1.00	14.72	8	ATOM	931	O	VAL	A 118	57.660	23.097	43.823	1.00	9.23	8
ATOM	879	OE2	GLU	A 111	49.218	41.958	54.436	1.00	15.89	8	ATOM	932	N	ASH	A 119	57.381	20.998	44.492	1.00	8.84	7
ATOM	880	C	GLU	A 111	54.697	40.516	52.799	1.00	12.41	6	ATOM	933	CA	ASH	A 119	57.701	20.403	43.206	1.00	8.20	6
ATOM	881	O	GLU	A 111	55.011	39.715	51.878	1.00	12.71	7	ATOM	934	CB	ASH	A 119	57.911	18.914	43.534	1.00	7.82	6
ATOM	882	N	ASP	A 112	55.284	40.485	53.981	1.00	12.71	7	ATOM	935	CG	ASH	A 119	58.248	18.097	42.289	1.00	8.10	6
ATOM	883	CA	ASP	A 112	56.344	39.543	54.283	1.00	13.23	6	ATOM	936	CO1	ASH	A 119	58.084	18.636	41.177	1.00	7.16	8
ATOM	884	CB	ASP	A 112	57.290	39.993	55.380	1.00	18.18	6	ATOM	937	MO2	ASH	A 119	58.706	16.848	42.386	1.00	6.98	7
ATOM	885	CG	ASP	A 112	58.008	41.297	55.120	1.00	21.75	6	ATOM	938	C	ASH	A 119	56.553	20.692	42.242	1.00	7.98	6
ATOM	886	CO1	ASP	A 112	58.435	41.747	54.039	1.00	23.40	8	ATOM	939	O	ASH	A 119	55.382	20.414	42.482	1.00	7.64	8
ATOM	887	CO2	ASP	A 112	58.189	42.024	56.128	1.00	24.60	8	ATOM	940	N	PRO	A 120	56.833	21.326	41.094	1.00	8.04	7
ATOM	888	C	ASP	A 112	55.666	38.250	54.730	1.00	13.29	6	ATOM	941	CD	PRO	A 120	58.207	21.735	40.728	1.00	8.00	6
ATOM	889	O	ASP	A 112	54.802	38.272	55.608	1.00	13.60	8	ATOM	942	CA	PRO	A 120	55.849	21.704	40.088	1.00	8.27	6
ATOM	890	N	VAL	A 113	56.015	37.098	54.155	1.00	13.04	7	ATOM	943	CG	PRO	A 120	56.609	22.404	38.938	1.00	8.21	6
ATOM	891	CA	VAL	A 113	55.381	35.819	54.410	1.00	12.72	6	ATOM	944	CG	PRO	A 120	57.980	22.618	39.530	1.00	8.16	6
ATOM	892	CB	VAL	A 113	54.466	35.495	53.205	1.00	13.86	6	ATOM	945	C	PRO	A 120	55.032	20.526	39.601	1.00	8.65	6
ATOM	893	CG1	VAL	A 113	53.650	34.192	53.418	1.00	14.55	6	ATOM	946	O	PRO	A 120	53.858	20.633	39.275	1.00	8.69	8
ATOM	894	CG2	VAL	A 113	53.423	36.541	52.806	1.00	13.68	6	ATOM	947	N	ALA	A 121	55.648	19.337	39.540	1.00	9.00	7
ATOM	895	C	VAL	A 113	56.407	34.721	54.511	1.00	12.52	6	ATOM	948	CA	ALA	A 121	54.977	18.104	39.122	1.00	9.39	6
ATOM	896	O	VAL	A 113	57.412	34.768	53.765	1.00	12.66	8	ATOM	949	CB	ALA	A 121	55.976	17.215	38.324	1.00	9.49	6
ATOM	897	N	THR	A 114	56.238	33.728	55.355	1.00	12.21	7	ATOM	950	C	ALA	A 121	54.374	17.315	40.267	1.00	9.46	6
ATOM	898	CA	THR	A 114	57.167	32.595	55.443	1.00	11.87	6	ATOM	951	O	ALA	A 121	53.644	16.327	40.066	1.00	9.60	8
ATOM	899	CB	THR	A 114	57.212	31.961	56.800	1.00	12.24	6	ATOM	952	N	ASH	A 122	54.624	17.656	41.537	1.00	9.45	7
ATOM	900	OG1	THR	A 114	57.602	32.955	57.741	1.00	14.04	8	ATOM	953	CA	ASH	A 122	54.040	16.971	42.679	1.00	9.32	7
ATOM	901	CG2	THR	A 114	58.195	30.781	56.909	1.00	10.63	6	ATOM	954	CB	ASH	A 122	54.881	15.802	43.207	1.00	10.30	6

ATOM	955	CG	ASN A 122	54.009	15.067	44.180	1.00	13.39	6
ATOM	956	NO1 ASN A 122	53.085	15.591	44.786	1.00	13.50	8	
ATOM	957	NO2 ASN A 122	54.211	13.733	44.357	1.00	16.10	7	
ATOM	958	C	ASN A 122	53.936	18.050	43.742	1.00	9.22	6
ATOM	959	O	ASN A 122	54.881	18.130	44.566	1.00	9.02	8
ATOM	960	N	ARG A 123	52.869	18.855	43.722	1.00	9.27	7
ATOM	961	CA	ARG A 123	52.764	19.983	44.684	1.00	9.23	6
ATOM	962	CB	ARG A 123	51.675	20.969	44.227	1.00	7.86	6
ATOM	963	CG	ARG A 123	52.067	21.766	42.991	1.00	6.67	6
ATOM	964	CD	ARG A 123	51.511	21.080	41.764	1.00	6.95	6
ATOM	965	HE	ARG A 123	51.759	21.959	40.604	1.00	9.73	7
ATOM	966	C2	ARG A 123	50.906	22.937	40.275	1.00	10.25	6
ATOM	967	NH1	ARG A 123	49.828	23.054	41.044	1.00	9.79	7
ATOM	968	NH2	ARG A 123	51.000	23.793	39.273	1.00	10.20	7
ATOM	969	C	ARG A 123	52.593	19.557	46.158	1.00	9.23	6
ATOM	970	O	ARG A 123	52.622	20.374	47.085	1.00	8.71	8
ATOM	971	N	ASN A 124	52.408	18.256	46.379	1.00	9.56	7
ATOM	972	CA	ASN A 124	52.351	17.706	47.712	1.00	10.31	6
ATOM	973	CG	ASN A 124	50.275	16.347	47.455	1.00	14.21	6
ATOM	974	CD	ASN A 124	49.565	17.271	47.867	1.00	14.26	8
ATOM	975	NO1 ASN A 124	53.796	15.391	46.590	1.00	16.51	7	
ATOM	976	NO2 ASN A 124	53.926	17.342	49.439	1.00	10.76	6	
ATOM	977	O	ASN A 124	56.872	17.660	47.433	1.00	10.85	8
ATOM	978	N	GLN A 125	56.223	17.549	47.925	1.00	11.21	6
ATOM	979	CA	GLN A 125	57.169	16.823	46.919	1.00	9.50	6
ATOM	980	CB	GLN A 125	58.582	16.600	47.498	1.00	8.17	6
ATOM	981	CG	GLN A 125	59.184	16.310	45.207	1.00	8.01	6
ATOM	982	CD	GLN A 125	59.566	16.199	46.402	1.00	6.56	8
ATOM	983	OE1 GLN A 125	59.184	16.310	45.207	1.00	6.20	7	
ATOM	984	OE2 GLN A 125	60.762	15.784	46.738	1.00	6.20	7	
ATOM	985	C	GLN A 125	56.871	18.915	48.156	1.00	11.48	6
ATOM	986	O	GLN A 125	56.960	19.609	47.146	1.00	11.44	8
ATOM	987	N	GLU A 126	57.345	19.217	49.360	1.00	11.79	7
ATOM	988	CA	GLU A 126	58.053	20.468	49.610	1.00	12.46	6
ATOM	989	CB	GLU A 126	58.042	20.856	51.115	1.00	11.31	6
ATOM	990	CG	GLU A 126	56.589	20.799	51.582	1.00	12.45	6
ATOM	991	CD	GLU A 126	56.371	21.288	52.993	1.00	13.36	6
ATOM	992	OE1 GLU A 126	57.329	21.471	53.748	1.00	13.22	8	
ATOM	993	OE2 GLU A 126	55.214	21.519	53.374	1.00	14.72	8	
ATOM	994	C	GLU A 126	59.513	20.293	49.195	1.00	13.18	6
ATOM	995	O	GLU A 126	60.198	19.292	48.513	1.00	12.98	8
ATOM	996	N	THR A 127	60.045	21.216	48.430	1.00	14.11	7
ATOM	997	CA	THR A 127	61.407	21.048	47.954	1.00	15.19	6
ATOM	998	CB	THR A 127	61.487	21.193	46.420	1.00	14.68	6
ATOM	999	CG	THR A 127	60.732	22.349	46.071	1.00	15.49	8
ATOM	1000	OC1 THR A 127	60.902	19.957	45.774	1.00	13.94	6	
ATOM	1001	OC2 THR A 127	62.377	21.993	48.614	1.00	16.26	6	
ATOM	1002	C	THR A 127	63.552	21.851	48.263	1.00	16.67	8
ATOM	1003	O	THR A 127	62.015	22.892	49.503	1.00	16.75	7
ATOM	1004	N	SER A 128	63.000	23.747	50.125	1.00	17.24	6
ATOM	1005	CA	SER A 128	63.016	25.141	49.511	1.00	15.04	6
ATOM	1006	CB	SER A 128	61.873	25.859	49.965	1.00	13.39	8
ATOM	1007	OG	SER A 128						
ATOM	1008	C	SER A 128	62.420	23.784	51.617	1.00	18.11	6
ATOM	1009	O	SER A 128	61.842	23.256	52.161	1.00	17.96	8
ATOM	1010	N	GLU A 129	63.523	24.444	52.326	1.00	18.90	7
ATOM	1011	CA	GLU A 129	63.395	24.747	53.735	1.00	19.85	6
ATOM	1012	CB	GLU A 129	64.718	25.038	54.440	1.00	27.78	6
ATOM	1013	CG	GLU A 129	64.794	24.360	55.817	1.00	35.30	6
ATOM	1014	CD	GLU A 129	65.311	22.937	55.587	1.00	40.42	6
ATOM	1015	OE1 GLU A 129	66.375	22.846	54.891	1.00	43.75	8	
ATOM	1016	OE2 GLU A 129	64.637	21.983	56.055	1.00	42.88	8	
ATOM	1017	C	GLU A 129	62.566	26.060	53.737	1.00	19.69	8
ATOM	1018	O	GLU A 129	62.573	26.773	52.713	1.00	19.50	8
ATOM	1019	N	GLU A 130	61.925	26.390	54.849	1.00	19.52	7
ATOM	1020	CA	GLU A 130	61.150	27.612	54.769	1.00	19.43	6
ATOM	1021	CB	GLU A 130	60.090	27.530	55.847	1.00	23.57	6
ATOM	1022	CG	GLU A 130	60.633	27.773	57.215	1.00	26.39	6
ATOM	1023	CD	GLU A 130	59.542	27.368	58.202	1.00	29.94	6
ATOM	1024	OE1 GLU A 130	59.493	28.140	59.202	1.00	33.34	8	
ATOM	1025	OE2 GLU A 130	58.779	26.388	58.051	1.00	30.50	6	
ATOM	1026	C	GLU A 130	61.988	28.851	54.837	1.00	18.97	6
ATOM	1027	O	GLU A 130	63.023	28.894	55.454	1.00	19.04	8
ATOM	1028	N	TYR A 131	61.506	29.854	54.117	1.00	18.45	7
ATOM	1029	CA	TYR A 131	62.186	31.164	54.098	1.00	17.87	6
ATOM	1030	CB	TYR A 131	63.336	31.254	53.126	1.00	18.14	6
ATOM	1031	CG	TYR A 131	63.123	31.022	51.656	1.00	18.56	6
ATOM	1032	CD	TYR A 131	63.015	32.108	50.786	1.00	18.80	6
ATOM	1033	OE1 TYR A 131	62.837	31.915	49.415	1.00	18.78	6	
ATOM	1034	OE2 TYR A 131	63.053	29.741	51.125	1.00	18.56	6	
ATOM	1035	C2 TYR A 131	62.856	29.566	47.772	1.00	18.73	6	
ATOM	1036	OM TYR A 131	62.753	30.638	48.908	1.00	18.74	6	
ATOM	1037	C	TYR A 131	61.150	32.287	53.841	1.00	17.13	6
ATOM	1038	O	TYR A 131	59.992	32.053	53.530	1.00	16.72	8
ATOM	1039	N	TYR A 131	61.601	33.503	54.011	1.00	16.51	7
ATOM	1040	N	GLN A 132	60.855	34.718	53.865	1.00	16.10	6
ATOM	1041	CA	GLN A 132	61.459	35.882	54.723	1.00	22.79	6
ATOM	1042	CB	GLN A 132	60.607	35.969	55.997	1.00	29.13	6
ATOM	1043	CG	GLN A 132	61.036	34.850	56.938	1.00	33.56	6
ATOM	1044	CD	GLN A 132	62.246	34.859	57.308	1.00	37.13	8
ATOM	1045	OE1 GLN A 132	60.138	33.934	57.337	1.00	34.32	7	
ATOM	1046	OE2 GLN A 132	60.810	35.316	52.481	1.00	15.05	6	
ATOM	1047	C	GLN A 132	61.881	35.620	51.931	1.00	15.27	8
ATOM	1048	O	GLN A 132	59.589	35.505	51.972	1.00	13.86	7
ATOM	1049	N	ILE A 133	59.481	36.102	50.631	1.00	12.62	6
ATOM	1050	CA	ILE A 133	58.828	35.111	49.616	1.00	11.38	6
ATOM	1051	CB	ILE A 133	59.610	33.787	49.649	1.00	9.01	6
ATOM	1052	CG	ILE A 133	57.374	34.744	49.978	1.00	11.33	6
ATOM	1053	CO1 ILE A 133	56.601	33.908	48.958	1.00	11.24	6	
ATOM	1054	CO2 ILE A 133	58.652	37.381	50.761	1.00	11.82	6	
ATOM	1055	C	ILE A 133	58.026	37.593	51.790	1.00	11.18	8
ATOM	1056	O	ILE A 133	58.611	38.192	49.709	1.00	11.45	7
ATOM	1057	N	LYS A 134	57.737	39.379	49.674	1.00	11.11	6
ATOM	1058	CA	LYS A 134	57.737	39.379	49.674	1.00	11.11	6
ATOM	1059	CB	LYS A 134	58.443	40.661	49.331	1.00	12.71	6
ATOM	1060	CG	LYS A 134	59.019	41.223	50.642	1.00	15.80	6

ATOM	1061	CD	LYS A 134	59.998	42.325	50.294	1.00	19.11	6	ATOM	1114	CG	ARG A 140	45.059	48.594	50.380	1.00	22.69	6
ATOM	1062	CE	LYS A 134	59.652	43.476	51.253	1.00	22.58	6	ATOM	1115	CD	ARG A 140	45.796	48.583	51.753	1.00	27.78	6
ATOM	1063	N2	LYS A 134	59.863	42.966	52.656	1.00	24.21	7	ATOM	1116	NE	ARG A 140	47.197	48.785	51.626	1.00	32.35	7
ATOM	1064	C	LYS A 134	56.683	39.046	48.618	1.00	10.75	6	ATOM	1117	C2	ARG A 140	48.476	48.985	51.487	1.00	34.38	6
ATOM	1065	O	LYS A 134	57.075	38.997	47.439	1.00	10.72	8	ATOM	1118	WH1	ARG A 140	48.873	49.714	50.421	1.00	34.62	7
ATOM	1066	H	ALA A 135	55.444	38.754	48.993	1.00	10.26	7	ATOM	1119	WH2	ARG A 140	49.440	48.518	52.329	1.00	34.86	7
ATOM	1067	CA	ALA A 135	54.411	38.356	48.066	1.00	9.82	6	ATOM	1120	C	ARG A 140	41.766	48.037	49.205	1.00	11.28	6
ATOM	1068	CB	ALA A 135	53.713	37.071	48.552	1.00	8.45	6	ATOM	1121	O	ARG A 140	40.965	48.699	49.916	1.00	11.54	8
ATOM	1069	C	ALA A 135	53.360	39.428	47.868	1.00	9.62	6	ATOM	1122	N	PHE A 141	41.672	47.993	47.908	1.00	10.83	7
ATOM	1070	O	ALA A 135	53.052	40.158	48.834	1.00	9.91	8	ATOM	1123	CA	PHE A 141	40.554	48.658	47.231	1.00	10.94	6
ATOM	1071	N	TRP A 136	52.718	39.492	46.672	1.00	9.28	7	ATOM	1124	CB	PHE A 141	39.237	47.897	47.618	1.00	8.15	6
ATOM	1072	CA	TRP A 136	51.676	40.473	46.354	1.00	8.76	6	ATOM	1125	CG	PHE A 141	39.346	46.381	47.561	1.00	6.78	6
ATOM	1073	CG	TRP A 136	51.683	40.690	44.846	1.00	9.45	6	ATOM	1126	CD1	PHE A 141	39.041	45.616	48.673	1.00	5.88	6
ATOM	1074	CG	TRP A 136	52.918	41.438	44.430	1.00	12.78	6	ATOM	1127	CD2	PHE A 141	39.793	45.725	46.453	1.00	5.72	6
ATOM	1075	CD2	TRP A 136	53.068	42.881	44.426	1.00	13.09	6	ATOM	1128	CE1	PHE A 141	39.150	44.225	48.627	1.00	6.27	6
ATOM	1076	CE2	TRP A 136	54.343	43.162	43.888	1.00	14.31	6	ATOM	1129	CE2	PHE A 141	39.930	44.318	46.407	1.00	5.00	6
ATOM	1077	CE3	TRP A 136	52.224	43.924	44.799	1.00	11.71	6	ATOM	1130	C2	PHE A 141	39.607	43.584	47.478	1.00	5.00	6
ATOM	1078	CD1	TRP A 136	54.098	40.924	43.934	1.00	13.83	6	ATOM	1131	C	PHE A 141	40.372	50.134	47.543	1.00	11.05	6
ATOM	1079	HE1	TRP A 136	54.954	41.951	43.599	1.00	13.49	7	ATOM	1132	O	PHE A 141	39.377	50.553	48.103	1.00	10.80	8
ATOM	1080	C22	TRP A 136	54.846	44.456	43.772	1.00	14.17	6	ATOM	1133	N	PRO A 142	41.402	50.934	47.254	1.00	11.32	7
ATOM	1081	C23	TRP A 136	52.680	45.213	44.627	1.00	12.36	6	ATOM	1134	CD	PRO A 142	42.645	50.440	46.634	1.00	11.43	6
ATOM	1082	CH2	TRP A 136	53.971	45.463	44.144	1.00	13.78	6	ATOM	1135	CA	PRO A 142	41.462	52.384	47.515	1.00	11.27	6
ATOM	1083	C	TRP A 136	50.338	39.995	46.811	1.00	8.40	6	ATOM	1136	CD	PRO A 142	42.900	52.829	47.190	1.00	11.50	6
ATOM	1084	O	TRP A 136	49.535	39.452	46.046	1.00	8.39	8	ATOM	1137	CG	PRO A 142	43.300	51.728	46.191	1.00	11.48	6
ATOM	1085	N	THR A 137	50.028	40.192	48.086	1.00	8.12	7	ATOM	1138	C	PRO A 142	40.424	53.179	46.766	1.00	11.03	6
ATOM	1086	CA	THR A 137	48.844	39.707	48.761	1.00	7.75	6	ATOM	1139	O	PRO A 142	39.933	54.100	47.431	1.00	11.24	8
ATOM	1087	CB	THR A 137	49.275	38.704	49.884	1.00	7.93	6	ATOM	1140	N	GLY A 143	39.984	52.964	45.545	1.00	10.61	7
ATOM	1088	CG1	THR A 137	50.351	39.218	50.701	1.00	8.77	8	ATOM	1141	CA	GLY A 143	38.950	53.703	44.905	1.00	10.26	6
ATOM	1089	CG2	THR A 137	49.847	37.387	49.327	1.00	8.10	6	ATOM	1142	C	GLY A 143	37.544	53.272	45.330	1.00	10.29	6
ATOM	1090	C	THR A 137	48.040	40.772	49.490	1.00	7.59	6	ATOM	1143	O	GLY A 143	36.578	54.011	45.134	1.00	10.11	8
ATOM	1091	O	THR A 137	47.063	40.370	50.112	1.00	7.09	8	ATOM	1144	N	ARG A 144	37.337	52.102	45.941	1.00	10.41	7
ATOM	1092	N	ASP A 138	48.425	42.026	49.486	1.00	7.55	7	ATOM	1145	CA	ARG A 144	36.034	51.630	46.365	1.00	10.66	6
ATOM	1093	CA	ASP A 138	47.680	43.038	50.221	1.00	7.91	6	ATOM	1146	CB	ARG A 144	35.855	50.122	46.046	1.00	6.45	6
ATOM	1094	CB	ASP A 138	48.667	44.060	50.793	1.00	10.34	6	ATOM	1147	CG	ARG A 144	34.545	49.572	46.609	1.00	6.59	6
ATOM	1095	CG	ASP A 138	48.054	45.085	51.742	1.00	14.50	6	ATOM	1148	CD	ARG A 144	34.074	48.222	46.139	1.00	6.10	6
ATOM	1096	OO1	ASP A 138	46.820	45.294	51.881	1.00	14.46	8	ATOM	1149	NE	ARG A 144	35.003	47.110	46.197	1.00	7.45	7
ATOM	1097	OO2	ASP A 138	48.865	45.781	52.416	1.00	16.18	8	ATOM	1150	C2	ARG A 144	35.062	46.377	47.500	1.00	7.53	6
ATOM	1098	C	ASP A 138	46.627	43.671	49.316	1.00	8.01	6	ATOM	1151	WH1	ARG A 144	35.983	45.402	47.626	1.00	8.54	7
ATOM	1099	O	ASP A 138	47.039	44.379	48.405	1.00	7.97	8	ATOM	1152	WH2	ARG A 144	34.219	46.599	48.511	1.00	6.60	7
ATOM	1100	N	PHE A 139	45.334	43.427	49.520	1.00	8.44	7	ATOM	1153	C	ARG A 144	35.736	51.908	47.869	1.00	11.31	6
ATOM	1101	CA	PHE A 139	44.208	44.016	48.652	1.00	9.00	6	ATOM	1154	O	ARG A 144	34.643	52.176	48.348	1.00	11.05	8
ATOM	1102	CB	PHE A 139	43.394	43.011	47.964	1.00	7.03	6	ATOM	1155	N	GLY A 145	36.813	51.804	48.658	1.00	11.78	7
ATOM	1103	CG	PHE A 139	44.078	42.176	46.892	1.00	8.72	6	ATOM	1156	CA	GLY A 145	36.758	51.954	50.104	1.00	12.35	6
ATOM	1104	CD1	PHE A 139	44.948	41.138	47.287	1.00	7.30	6	ATOM	1157	C	GLY A 145	35.922	50.757	50.584	1.00	12.97	6
ATOM	1105	CD2	PHE A 139	43.835	42.398	45.538	1.00	7.95	6	ATOM	1158	O	GLY A 145	36.169	49.601	50.164	1.00	13.33	8
ATOM	1106	CE1	PHE A 139	45.600	40.359	46.350	1.00	8.84	6	ATOM	1159	N	ASN A 146	34.906	51.057	51.416	1.00	12.95	7
ATOM	1107	CE2	PHE A 139	44.469	41.605	44.591	1.00	8.85	6	ATOM	1160	CA	ASN A 146	34.070	49.991	51.970	1.00	12.83	6
ATOM	1108	C2	PHE A 139	45.335	40.593	44.979	1.00	9.11	6	ATOM	1161	CB	ASN A 146	33.889	50.195	53.493	1.00	15.58	6
ATOM	1109	C	PHE A 139	45.461	44.987	49.487	1.00	9.73	6	ATOM	1162	CG	ASN A 146	35.151	49.936	54.288	1.00	19.40	6
ATOM	1110	O	PHE A 139	42.707	44.536	50.343	1.00	9.71	8	ATOM	1163	CD1	ASN A 146	36.085	49.159	53.989	1.00	20.79	8
ATOM	1111	N	ARG A 140	43.599	46.294	49.178	1.00	10.52	7	ATOM	1164	WD2	ASN A 146	35.264	50.678	55.410	1.00	20.44	7
ATOM	1112	CA	ARG A 140	42.823	47.246	49.985	1.00	11.46	6	ATOM	1165	C	ASN A 146	32.689	49.855	51.336	1.00	12.13	6
ATOM	1113	CB	ARG A 140	43.647	48.263	50.745	1.00	17.79	6	ATOM	1166	O	ASN A 146	31.905	49.168	52.002	1.00	12.08	8

ATOM	1167	N	THR A 147	32.491	50.456	50.175	1.00	11.60	7
ATOM	1168	CA	THR A 147	31.200	50.351	49.487	1.00	11.26	6
ATOM	1169	CB	THR A 147	31.164	51.128	48.161	1.00	11.45	6
ATOM	1170	OG1	THR A 147	31.709	52.445	48.360	1.00	12.12	8
ATOM	1171	CG2	THR A 147	29.782	51.325	47.548	1.00	9.27	6
ATOM	1172	C	THR A 147	30.895	48.884	49.247	1.00	11.00	6
ATOM	1173	O	THR A 147	31.757	48.136	48.721	1.00	11.07	8
ATOM	1174	H	THR A 148	29.718	48.430	49.662	1.00	10.51	7
ATOM	1175	CA	THR A 148	29.245	47.066	49.538	1.00	10.34	6
ATOM	1176	CB	THR A 148	29.308	46.455	48.113	1.00	10.35	6
ATOM	1177	CG	THR A 148	28.798	47.326	46.967	1.00	9.97	6
ATOM	1178	CD1	THR A 148	29.649	47.666	45.916	1.00	9.49	6
ATOM	1179	CE1	THR A 148	29.177	48.430	44.845	1.00	9.11	6
ATOM	1180	CD2	THR A 148	27.474	47.843	46.971	1.00	9.73	6
ATOM	1181	CE2	THR A 148	27.067	48.636	45.925	1.00	9.48	6
ATOM	1182	CZ	THR A 148	27.896	48.916	44.844	1.00	8.99	6
ATOM	1183	OH	THR A 148	27.441	49.705	43.833	1.00	8.37	8
ATOM	1184	C	THR A 148	29.940	46.030	50.426	1.00	10.22	6
ATOM	1185	O	THR A 149	29.299	45.054	50.827	1.00	10.08	8
ATOM	1186	N	SER A 149	31.224	46.159	50.757	1.00	10.07	7
ATOM	1187	CA	SER A 149	31.879	45.141	51.584	1.00	9.72	6
ATOM	1188	CB	SER A 149	32.256	43.886	50.787	1.00	9.55	6
ATOM	1189	CG	SER A 149	33.396	43.185	51.181	1.00	8.96	8
ATOM	1190	C	SER A 149	33.141	43.735	52.164	1.00	9.63	8
ATOM	1191	O	SER A 149	33.897	46.334	51.423	1.00	9.31	8
ATOM	1192	H	ASP A 150	33.270	45.588	53.502	1.00	9.75	7
ATOM	1193	CA	ASP A 150	34.497	46.155	54.053	1.00	9.98	6
ATOM	1194	CB	ASP A 150	34.153	46.816	55.365	1.00	13.89	6
ATOM	1195	CG	ASP A 150	33.646	45.849	56.403	1.00	17.64	6
ATOM	1196	CD1	ASP A 150	33.340	44.644	56.213	1.00	18.84	8
ATOM	1197	CD2	ASP A 150	33.560	46.260	57.579	1.00	20.98	8
ATOM	1198	C	ASP A 150	35.545	45.049	54.125	1.00	9.95	6
ATOM	1199	O	ASP A 150	36.570	45.334	54.761	1.00	10.38	8
ATOM	1200	N	PHE A 151	35.472	43.865	53.561	1.00	9.49	7
ATOM	1201	CA	PHE A 151	36.518	42.860	53.467	1.00	8.88	6
ATOM	1202	CB	PHE A 151	35.932	41.523	53.167	1.00	10.40	6
ATOM	1203	CG	PHE A 151	36.761	40.297	53.405	1.00	12.18	6
ATOM	1204	CD1	PHE A 151	36.689	39.627	54.620	1.00	14.04	6
ATOM	1205	CD2	PHE A 151	37.623	39.804	52.455	1.00	12.75	6
ATOM	1206	CE1	PHE A 151	37.481	38.471	54.849	1.00	15.14	6
ATOM	1207	CE2	PHE A 151	38.380	38.647	52.644	1.00	12.08	6
ATOM	1208	CZ	PHE A 151	38.308	37.976	53.869	1.00	13.39	6
ATOM	1209	C	PHE A 151	37.748	43.217	52.864	1.00	8.54	6
ATOM	1210	O	PHE A 151	37.762	43.556	51.675	1.00	8.21	8
ATOM	1211	N	LYS A 152	36.899	43.119	53.477	1.00	8.21	7
ATOM	1212	CA	LYS A 152	40.228	43.377	52.979	1.00	8.62	6
ATOM	1213	CB	LYS A 152	40.989	44.385	53.849	1.00	10.86	6
ATOM	1214	CG	LYS A 152	40.384	45.787	54.073	1.00	11.07	6
ATOM	1215	CD	LYS A 152	39.941	46.481	52.798	1.00	11.11	6
ATOM	1216	CE	LYS A 152	39.350	47.850	53.236	1.00	12.45	6
ATOM	1217	H2	LYS A 152	38.434	48.440	52.290	1.00	15.39	7
ATOM	1218	C	LYS A 152	41.038	42.082	52.958	1.00	8.53	6
ATOM	1219	O	LYS A 152	40.938	41.290	53.892	1.00	8.53	8
ATOM	1220	N	TRP A 153	41.841	41.875	41.841	1.00	8.13	7
ATOM	1221	CA	TRP A 153	42.565	40.644	51.805	1.00	7.85	6
ATOM	1222	CB	TRP A 153	42.567	40.241	50.293	1.00	6.88	6
ATOM	1223	CG	TRP A 153	41.174	39.851	49.872	1.00	6.70	6
ATOM	1224	CD2	TRP A 153	40.681	38.522	49.679	1.00	6.38	6
ATOM	1225	CE2	TRP A 153	39.330	38.637	49.270	1.00	7.85	6
ATOM	1226	CE3	TRP A 153	41.225	37.236	49.779	1.00	6.59	6
ATOM	1227	CD1	TRP A 153	40.139	40.695	49.600	1.00	6.77	6
ATOM	1228	WE1	TRP A 153	39.018	39.986	49.233	1.00	6.86	7
ATOM	1229	C22	TRP A 153	38.542	37.504	48.986	1.00	7.93	6
ATOM	1230	C23	TRP A 153	40.477	36.113	49.452	1.00	7.12	6
ATOM	1231	CM2	TRP A 153	39.128	36.250	49.081	1.00	8.55	6
ATOM	1232	C	TRP A 153	44.014	40.738	52.256	1.00	7.70	6
ATOM	1233	O	TRP A 153	44.633	41.770	52.009	1.00	7.54	8
ATOM	1234	N	HIS A 154	44.568	39.706	52.892	1.00	7.67	7
ATOM	1235	CA	HIS A 154	45.937	39.586	53.334	1.00	7.24	6
ATOM	1236	CB	HIS A 154	46.112	39.730	54.859	1.00	7.92	6
ATOM	1237	CG	HIS A 154	45.804	41.145	55.233	1.00	8.88	6
ATOM	1238	CD2	HIS A 154	44.674	41.660	55.765	1.00	9.84	6
ATOM	1239	WD1	HIS A 154	46.672	42.197	55.006	1.00	10.11	7
ATOM	1240	ME1	HIS A 154	46.113	43.304	55.428	1.00	10.55	6
ATOM	1241	ME2	HIS A 154	44.890	43.016	55.840	1.00	10.76	7
ATOM	1242	C	HIS A 154	46.508	38.207	52.960	1.00	6.90	6
ATOM	1243	O	HIS A 154	45.778	37.294	52.603	1.00	6.75	8
ATOM	1244	N	TRP A 155	47.839	38.056	53.102	1.00	6.82	7
ATOM	1245	CA	TRP A 155	48.508	36.802	52.800	1.00	6.92	6
ATOM	1246	CB	TRP A 155	49.994	36.800	53.254	1.00	6.54	6
ATOM	1247	CG	TRP A 155	50.190	36.808	54.726	1.00	6.55	6
ATOM	1248	CD2	TRP A 155	50.282	35.636	55.575	1.00	7.16	6
ATOM	1249	CE2	TRP A 155	50.473	36.099	56.900	1.00	8.10	6
ATOM	1250	CE3	TRP A 155	50.261	34.254	55.319	1.00	7.58	6
ATOM	1251	CD1	TRP A 155	50.311	37.912	55.567	1.00	7.09	6
ATOM	1252	ME1	TRP A 155	50.496	37.495	56.870	1.00	7.83	7
ATOM	1253	C22	TRP A 155	50.582	35.208	57.972	1.00	9.47	6
ATOM	1254	C23	TRP A 155	50.372	33.377	56.355	1.00	8.70	6
ATOM	1255	CM2	TRP A 155	50.556	33.847	57.685	1.00	9.74	6
ATOM	1256	C	TRP A 155	47.807	35.600	53.420	1.00	6.90	6
ATOM	1257	O	TRP A 155	47.749	34.576	52.755	1.00	6.82	8
ATOM	1258	N	TYR A 156	47.293	35.659	54.655	1.00	6.91	7
ATOM	1259	CA	TYR A 156	46.692	34.492	55.283	1.00	6.91	6
ATOM	1260	CB	TYR A 156	46.619	34.685	56.813	1.00	7.50	6
ATOM	1261	CG	TYR A 156	46.056	36.003	57.270	1.00	8.16	6
ATOM	1262	CD1	TYR A 156	44.665	36.114	57.420	1.00	8.66	6
ATOM	1263	CE1	TYR A 156	44.049	37.302	57.839	1.00	8.68	6
ATOM	1264	CD2	TYR A 156	46.829	37.094	57.597	1.00	8.54	6
ATOM	1265	CE2	TYR A 156	46.254	38.298	58.052	1.00	8.83	6
ATOM	1266	CZ	TYR A 156	44.870	38.365	58.159	1.00	8.97	6
ATOM	1267	OH	TYR A 156	44.271	39.510	58.597	1.00	9.48	8
ATOM	1268	C	TYR A 156	45.351	34.041	54.691	1.00	6.48	6
ATOM	1269	O	TYR A 156	44.907	32.991	55.146	1.00	6.37	8
ATOM	1270	N	HIS A 157	44.751	34.691	53.719	1.00	5.96	7
ATOM	1271	CA	HIS A 157	43.567	34.321	53.016	1.00	5.71	6
ATOM	1272	CB	HIS A 157	42.768	35.566	52.552	1.00	5.00	6

ATOM	1273	CG	HIS A 157	42.236	36.398	53.732	1.00	5.00	6
ATOM	1274	CD2	HIS A 157	41.620	36.018	54.866	1.00	5.00	6
ATOM	1275	ND1	HIS A 157	42.426	37.765	53.793	1.00	5.10	7
ATOM	1276	CE1	HIS A 157	41.880	38.216	54.935	1.00	6.49	6
ATOM	1277	HE2	HIS A 157	41.398	37.147	55.588	1.00	5.12	7
ATOM	1278	C	HIS A 157	43.896	33.473	51.753	1.00	5.75	6
ATOM	1279	O	HIS A 157	43.028	33.056	50.978	1.00	5.63	8
ATOM	1280	H	PIE A 158	45.182	33.311	51.471	1.00	5.60	7
ATOM	1281	CA	PIE A 158	45.722	32.597	50.312	1.00	5.84	6
ATOM	1282	CB	PIE A 158	46.578	33.527	49.412	1.00	5.00	6
ATOM	1283	CG	PIE A 158	45.867	34.784	48.992	1.00	5.00	6
ATOM	1284	CD1	PIE A 158	46.099	35.994	49.658	1.00	5.00	6
ATOM	1285	CD2	PIE A 158	44.494	37.129	48.230	1.00	5.00	6
ATOM	1286	CE1	PIE A 158	45.418	37.147	49.286	1.00	5.00	6
ATOM	1287	CE2	PIE A 158	44.300	35.931	47.568	1.00	5.36	6
ATOM	1288	CZ	PIE A 158	46.580	31.365	50.692	1.00	5.65	6
ATOM	1289	O	PHE A 158	47.192	31.311	51.800	1.00	5.98	8
ATOM	1290	O	PHE A 158	46.638	30.354	49.804	1.00	5.30	6
ATOM	1291	CA	ASP A 159	47.461	29.211	50.022	1.00	5.59	7
ATOM	1292	CB	ASP A 159	46.924	27.979	49.262	1.00	5.00	6
ATOM	1293	CG	ASP A 159	45.876	27.378	50.090	1.00	5.58	6
ATOM	1294	CG	ASP A 159	45.988	27.501	51.360	1.00	8.12	8
ATOM	1295	CD1	ASP A 159	44.852	26.813	49.700	1.00	5.00	8
ATOM	1296	CD2	ASP A 159	48.876	29.377	49.678	1.00	5.70	6
ATOM	1297	C	ASP A 159	49.808	28.719	49.999	1.00	6.04	8
ATOM	1298	O	ASP A 159	49.083	30.164	48.444	1.00	5.67	7
ATOM	1299	N	GLY A 160	50.438	30.251	47.914	1.00	6.24	6
ATOM	1300	CA	GLY A 160	50.472	31.296	46.798	1.00	6.82	6
ATOM	1301	C	GLY A 160	49.389	31.807	46.477	1.00	6.74	8
ATOM	1302	O	GLY A 160	51.622	31.520	46.224	1.00	7.20	7
ATOM	1303	N	ALA A 161	51.756	32.488	45.174	1.00	8.08	6
ATOM	1304	CA	ALA A 161	52.023	33.869	45.775	1.00	8.88	6
ATOM	1305	CB	ALA A 161	52.933	32.083	44.297	1.00	9.05	6
ATOM	1306	C	ALA A 161	53.582	31.055	44.591	1.00	8.86	8
ATOM	1307	O	ALA A 161	53.158	32.846	43.215	1.00	10.00	7
ATOM	1308	N	ASP A 162	54.278	32.418	42.372	1.00	11.36	6
ATOM	1309	CA	ASP A 162	53.786	32.031	40.983	1.00	15.10	6
ATOM	1310	CB	ASP A 162	53.111	33.242	40.352	1.00	19.35	6
ATOM	1311	CG	ASP A 162	52.930	34.331	40.947	1.00	19.47	8
ATOM	1312	CD1	ASP A 162	52.725	32.956	39.169	1.00	22.93	8
ATOM	1313	CD2	ASP A 162	55.381	33.455	42.149	1.00	11.95	6
ATOM	1314	C	ASP A 162	56.107	33.336	41.131	1.00	12.10	8
ATOM	1315	O	ASP A 162	55.489	34.435	43.048	1.00	12.03	7
ATOM	1316	N	TRP A 163	56.533	35.418	42.793	1.00	12.34	6
ATOM	1317	CA	TRP A 163	55.954	36.485	41.881	1.00	12.40	6
ATOM	1318	CB	TRP A 163	56.925	37.600	41.631	1.00	13.20	6
ATOM	1319	CG	TRP A 163	58.014	37.602	40.715	1.00	14.18	6
ATOM	1320	CD2	TRP A 163	58.646	38.869	40.826	1.00	15.32	6
ATOM	1321	CD2	TRP A 163	58.520	36.667	39.803	1.00	14.71	6
ATOM	1322	CE3	TRP A 163	56.950	38.813	42.745	1.00	13.62	6
ATOM	1323	CD1	TRP A 163	57.980	39.589	41.774	1.00	13.74	7
ATOM	1324	HE1	TRP A 163	59.757	39.243	40.036	1.00	16.07	6
ATOM	1325	C22	TRP A 163						
ATOM	1326	C23	TRP A 163						
ATOM	1327	CH2	TRP A 163						
ATOM	1328	C	TRP A 163						
ATOM	1329	O	TRP A 163						
ATOM	1330	N	ASP A 164						
ATOM	1331	CA	ASP A 164						
ATOM	1332	CB	ASP A 164						
ATOM	1333	CG	ASP A 164						
ATOM	1334	CD1	ASP A 164						
ATOM	1335	CD2	ASP A 164						
ATOM	1336	C	ASP A 164						
ATOM	1337	O	ASP A 164						
ATOM	1338	CA	GLU A 165						
ATOM	1339	CB	GLU A 165						
ATOM	1340	CG	GLU A 165						
ATOM	1341	CG	GLU A 165						
ATOM	1342	OE1	GLU A 165						
ATOM	1343	OE2	GLU A 165						
ATOM	1344	O	GLU A 165						
ATOM	1345	N	SER A 166						
ATOM	1346	CA	SER A 166						
ATOM	1347	CB	SER A 166						
ATOM	1348	CG	SER A 166						
ATOM	1349	CG	SER A 166						
ATOM	1350	OC	SER A 166						
ATOM	1351	C	SER A 166						
ATOM	1352	O	SER A 166						
ATOM	1353	N	ARG A 167						
ATOM	1354	CA	ARG A 167						
ATOM	1355	CB	ARG A 167						
ATOM	1356	CG	ARG A 167						
ATOM	1357	CD	ARG A 167						
ATOM	1358	NE	ARG A 167						
ATOM	1359	CZ	ARG A 167						
ATOM	1360	HH1	ARG A 167						
ATOM	1361	HH2	ARG A 167						
ATOM	1362	C	ARG A 167						
ATOM	1363	O	ARG A 167						
ATOM	1364	N	LYS A 168						
ATOM	1365	CA	LYS A 168						
ATOM	1366	CB	LYS A 168						
ATOM	1367	CG	LYS A 168						
ATOM	1368	CD	LYS A 168						
ATOM	1369	CE	LYS A 168						
ATOM	1370	HE	LYS A 168						
ATOM	1371	C	LYS A 168						
ATOM	1372	O	LYS A 168						
ATOM	1373	N	ILE A 169						
ATOM	1374	CA	ILE A 169						
ATOM	1375	CB	ILE A 169						
ATOM	1376	CG	ILE A 169						
ATOM	1377	CD	ILE A 169						
ATOM	1378	CD1	ILE A 169						

ATOM	1379	C	ILE	A	169	60.748	34.265	41.354	1.00	16.43	6
ATOM	1380	O	ILE	A	169	59.894	34.602	42.175	1.00	15.97	8
ATOM	1381	N	SER	A	170	60.458	33.469	40.342	1.00	16.39	7
ATOM	1382	CA	SER	A	170	59.209	32.808	40.120	1.00	16.32	6
ATOM	1383	CG	SER	A	170	58.830	32.767	38.642	1.00	16.20	6
ATOM	1384	OG	SER	A	170	57.519	32.181	38.607	1.00	22.81	8
ATOM	1385	C	SER	A	170	59.306	31.335	40.518	1.00	16.18	6
ATOM	1386	O	SER	A	170	60.106	30.999	39.908	1.00	16.17	8
ATOM	1387	N	ARG	A	171	58.531	30.882	41.508	1.00	15.84	7
ATOM	1388	CA	ARG	A	171	58.504	29.492	41.954	1.00	15.28	6
ATOM	1389	CB	ARG	A	171	59.448	29.168	43.104	1.00	17.32	6
ATOM	1390	CG	ARG	A	171	60.894	29.497	43.152	1.00	19.88	6
ATOM	1391	CD	ARG	A	171	61.825	28.448	42.555	1.00	23.48	6
ATOM	1392	NE	ARG	A	171	63.204	28.981	42.466	1.00	27.05	7
ATOM	1393	CZ	ARG	A	171	63.661	29.577	41.358	1.00	29.43	6
ATOM	1394	NH1	ARG	A	171	62.909	29.718	40.256	1.00	30.87	7
ATOM	1395	NH2	ARG	A	171	64.884	30.070	41.191	1.00	30.59	7
ATOM	1396	C	ARG	A	171	57.052	29.164	42.380	1.00	14.63	6
ATOM	1397	O	ARG	A	171	56.203	30.055	42.313	1.00	14.71	8
ATOM	1398	N	ILE	A	172	56.737	27.949	42.824	1.00	13.80	7
ATOM	1399	CA	ILE	A	172	55.389	27.671	43.336	1.00	13.02	6
ATOM	1400	CB	ILE	A	172	54.752	26.357	42.862	1.00	11.93	6
ATOM	1401	CG1	ILE	A	172	53.502	26.058	43.656	1.00	11.06	6
ATOM	1402	CG1	ILE	A	172	54.360	26.386	41.354	1.00	11.59	6
ATOM	1403	CD1	ILE	A	172	53.920	25.010	40.927	1.00	12.67	6
ATOM	1404	C	ILE	A	172	55.639	27.730	44.867	1.00	12.55	6
ATOM	1405	O	ILE	A	172	56.218	26.808	45.469	1.00	12.52	8
ATOM	1406	N	PHE	A	173	55.290	28.812	45.529	1.00	11.95	7
ATOM	1407	CA	PHE	A	173	55.464	28.982	46.956	1.00	11.52	6
ATOM	1408	CB	PHE	A	173	55.813	30.424	47.326	1.00	8.63	6
ATOM	1409	CG	PHE	A	173	57.088	30.932	46.719	1.00	8.19	6
ATOM	1410	CD1	PHE	A	173	57.085	31.843	45.697	1.00	6.97	6
ATOM	1411	CD2	PHE	A	173	58.313	30.470	47.211	1.00	8.07	6
ATOM	1412	CE1	PHE	A	173	58.277	32.307	45.123	1.00	8.69	6
ATOM	1413	CE2	PHE	A	173	59.512	30.949	46.686	1.00	8.72	6
ATOM	1414	C2	PHE	A	173	59.484	31.844	45.607	1.00	7.75	6
ATOM	1415	C	PHE	A	173	54.189	28.583	47.688	1.00	11.50	6
ATOM	1416	O	PHE	A	173	53.109	29.085	47.372	1.00	11.79	8
ATOM	1417	N	LYS	A	174	54.257	27.696	48.657	1.00	11.28	7
ATOM	1418	CA	LYS	A	174	53.185	27.303	49.524	1.00	11.02	6
ATOM	1419	CB	LYS	A	174	53.268	25.849	49.981	1.00	7.54	6
ATOM	1420	CG	LYS	A	174	52.045	25.443	50.770	1.00	6.03	6
ATOM	1421	CD	LYS	A	174	51.880	23.947	50.993	1.00	5.90	6
ATOM	1422	CE	LYS	A	174	53.109	23.439	51.713	1.00	6.00	6
ATOM	1423	N2	LYS	A	174	52.991	22.034	52.176	1.00	5.20	7
ATOM	1424	C	LYS	A	174	53.313	28.195	50.787	1.00	11.19	6
ATOM	1425	O	LYS	A	174	54.402	28.117	51.406	1.00	11.32	8
ATOM	1426	N	PHE	A	175	52.357	28.950	51.264	1.00	11.10	7
ATOM	1427	CA	PHE	A	175	52.555	29.759	52.486	1.00	11.23	6
ATOM	1428	CB	PHE	A	175	51.440	30.845	52.516	1.00	9.58	6
ATOM	1429	CG	PHE	A	175	51.497	31.920	51.427	1.00	9.11	6
ATOM	1430	CD1	PHE	A	175	50.410	32.806	51.283	1.00	8.73	6
ATOM	1431	CD2	PHE	A	175	52.569	32.097	50.557	1.00	7.13	6
ATOM	1432	CE1	PHE	A	175	50.443	33.823	50.320	1.00	7.64	6
ATOM	1433	CE2	PHE	A	175	52.585	33.103	49.614	1.00	6.81	6
ATOM	1434	C2	PHE	A	175	51.517	33.983	49.476	1.00	7.21	6
ATOM	1435	C	PHE	A	175	52.567	28.942	53.770	1.00	11.49	6
ATOM	1436	O	PHE	A	175	51.868	27.912	53.875	1.00	11.44	8
ATOM	1437	N	ARG	A	176	53.288	29.352	54.813	1.00	11.77	7
ATOM	1438	CA	ARG	A	176	53.328	28.725	56.129	1.00	12.20	6
ATOM	1439	CB	ARG	A	176	54.684	28.802	56.775	1.00	13.53	6
ATOM	1440	CG	ARG	A	176	55.768	27.776	56.372	1.00	14.88	6
ATOM	1441	CD	ARG	A	176	55.188	26.438	56.823	1.00	15.37	6
ATOM	1442	NE	ARG	A	176	56.133	25.355	56.737	1.00	15.69	7
ATOM	1443	CG	ARG	A	176	56.118	24.277	55.962	1.00	16.02	6
ATOM	1444	NH1	ARG	A	176	55.150	24.037	55.065	1.00	16.35	7
ATOM	1445	NH2	ARG	A	176	57.151	23.430	56.062	1.00	16.02	7
ATOM	1446	C	ARG	A	176	52.330	29.526	56.994	1.00	12.82	6
ATOM	1447	O	ARG	A	176	52.303	30.774	56.778	1.00	12.92	8
ATOM	1448	N	GLY	A	177	51.560	28.911	57.850	1.00	13.07	7
ATOM	1449	CA	GLY	A	177	50.590	29.656	58.637	1.00	13.84	6
ATOM	1450	C	GLY	A	177	49.736	28.715	59.449	1.00	14.51	6
ATOM	1451	O	GLY	A	177	50.056	27.482	59.489	1.00	15.11	8
ATOM	1452	N	GLU	A	178	48.649	29.125	60.069	1.00	14.47	7
ATOM	1453	CA	GLU	A	178	47.810	28.222	60.859	1.00	14.86	6
ATOM	1454	CB	GLU	A	178	46.912	29.021	61.833	1.00	15.74	6
ATOM	1455	CG	GLU	A	178	47.575	29.715	63.000	1.00	16.47	6
ATOM	1456	CG1	GLU	A	178	48.458	28.762	63.819	1.00	18.26	6
ATOM	1457	CE1	GLU	A	178	48.216	27.504	63.969	1.00	19.50	8
ATOM	1458	CE2	GLU	A	178	49.488	29.266	64.326	1.00	16.85	8
ATOM	1459	C	GLU	A	178	46.961	27.310	59.957	1.00	15.02	6
ATOM	1460	O	GLU	A	178	46.138	27.801	59.151	1.00	15.35	8
ATOM	1461	N	GLY	A	179	47.148	26.015	60.032	1.00	14.81	7
ATOM	1462	CA	GLY	A	179	46.450	25.042	59.221	1.00	14.68	6
ATOM	1463	C	GLY	A	179	46.692	25.221	57.702	1.00	14.28	6
ATOM	1464	O	GLY	A	179	45.709	24.906	56.979	1.00	14.54	8
ATOM	1465	N	LYS	A	180	47.854	25.708	57.243	1.00	13.43	7
ATOM	1466	CA	LYS	A	180	48.022	25.959	55.824	1.00	12.55	6
ATOM	1467	CB	LYS	A	180	49.163	26.955	55.631	1.00	11.48	6
ATOM	1468	CG	LYS	A	180	48.825	28.409	55.816	1.00	11.89	6
ATOM	1469	CD	LYS	A	180	47.710	28.914	54.938	1.00	9.28	6
ATOM	1470	CE	LYS	A	180	47.355	30.371	55.116	1.00	9.37	6
ATOM	1471	N2	LYS	A	180	46.097	30.683	54.339	1.00	9.60	7
ATOM	1472	C	LYS	A	180	48.271	24.676	55.037	1.00	12.15	6
ATOM	1473	O	LYS	A	180	49.150	23.919	55.465	1.00	12.30	8
ATOM	1474	N	ALA	A	181	47.571	24.402	53.925	1.00	11.19	7
ATOM	1475	CA	ALA	A	181	47.792	23.208	53.139	1.00	10.23	6
ATOM	1476	CB	ALA	A	181	47.183	21.975	53.825	1.00	8.27	6
ATOM	1477	C	ALA	A	181	47.120	23.287	51.761	1.00	9.57	6
ATOM	1478	O	ALA	A	181	46.125	23.952	51.862	1.00	8.95	8
ATOM	1479	N	TRP	A	182	47.457	22.762	50.604	1.00	8.86	7
ATOM	1480	CA	TRP	A	182	46.604	22.929	49.465	1.00	8.54	6
ATOM	1481	CB	TRP	A	182	47.232	22.145	48.309	1.00	6.73	6
ATOM	1482	CG	TRP	A	182	48.624	22.609	47.966	1.00	5.79	6
ATOM	1483	CD2	TRP	A	182	49.003	23.922	47.558	1.00	5.00	6
ATOM	1484	CE2	TRP	A	182	50.388	23.887	47.314	1.00	5.13	6

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1485	ATOM	CE3 TRP A 182	48.278	25.127	47.361	1.00	5.00	6
1486	ATOM	CD1 TRP A 182	49.768	21.861	48.002	1.00	5.63	6
1487	ATOM	WE1 TRP A 182	50.860	22.616	47.616	1.00	5.04	7
1488	ATOM	C22 TRP A 182	51.110	25.022	46.895	1.00	5.00	6
1489	ATOM	C23 TRP A 182	48.966	26.236	46.927	1.00	5.00	6
1490	ATOM	CH2 TRP A 182	50.378	26.186	46.723	1.00	5.00	6
1491	ATOM	C TRP A 182	45.218	22.348	46.787	1.00	8.52	6
1492	ATOM	O TRP A 182	45.029	21.400	50.552	1.00	8.24	8
1493	ATOM	H ASP A 183	44.187	22.939	49.183	1.00	8.61	7
1494	ATOM	CA ASP A 183	42.814	22.546	49.339	1.00	8.57	6
1495	ATOM	CB ASP A 183	41.746	23.407	48.669	1.00	7.64	6
1496	ATOM	CG ASP A 183	41.829	24.846	49.207	1.00	7.97	6
1497	ATOM	CD1 ASP A 183	42.136	25.011	50.384	1.00	5.19	8
1498	ATOM	CD2 ASP A 183	41.604	25.903	48.623	1.00	7.20	8
1499	ATOM	C ASP A 183	42.678	21.163	48.661	1.00	8.68	6
1500	ATOM	O ASP A 183	43.392	20.764	47.757	1.00	8.29	8
1501	ATOM	N TRP A 184	41.655	19.216	48.016	1.00	9.31	6
1502	ATOM	CA TRP A 184	41.337	19.216	48.016	1.00	9.31	6
1503	ATOM	CB TRP A 184	42.068	18.015	49.485	1.00	9.16	6
1504	ATOM	CG TRP A 184	41.858	16.719	48.816	1.00	9.24	6
1505	ATOM	CD2 TRP A 184	42.391	16.211	47.580	1.00	9.64	6
1506	ATOM	CE2 TRP A 184	41.870	14.896	47.384	1.00	9.60	6
1507	ATOM	CD1 TRP A 184	43.240	16.730	46.594	1.00	10.01	8
1508	ATOM	CE3 TRP A 184	41.009	15.713	49.300	1.00	10.78	6
1509	ATOM	WE1 TRP A 184	41.019	14.620	48.426	1.00	9.86	7
1510	ATOM	C22 TRP A 184	42.149	14.151	46.250	1.00	9.71	6
1511	ATOM	C23 TRP A 184	43.547	15.968	45.479	1.00	9.85	6
1512	ATOM	CH2 TRP A 184	43.008	14.693	45.314	1.00	9.96	6
1513	ATOM	C TRP A 184	39.766	18.960	48.936	1.00	9.70	6
1514	ATOM	O TRP A 184	39.093	19.322	49.789	1.00	10.01	8
1515	ATOM	H GLU A 185	39.594	18.432	47.785	1.00	9.88	7
1516	ATOM	CA GLU A 185	39.263	17.724	46.655	1.00	9.32	6
1517	ATOM	CB GLU A 185	38.201	16.707	46.321	1.00	11.19	6
1518	ATOM	CG GLU A 185	38.829	15.901	45.132	1.00	11.41	6
1519	ATOM	CD GLU A 185	38.070	14.631	44.814	1.00	13.77	6
1520	ATOM	OE1 GLU A 185	37.147	14.228	45.559	1.00	14.04	8
1521	ATOM	OE2 GLU A 185	38.349	14.001	43.768	1.00	14.41	8
1522	ATOM	C GLU A 185	39.394	18.759	45.479	1.00	8.78	6
1523	ATOM	O GLU A 185	38.591	19.636	45.294	1.00	8.92	8
1524	ATOM	N VAL A 186	40.502	18.566	44.792	1.00	8.34	7
1525	ATOM	CA VAL A 186	40.810	19.326	43.583	1.00	8.33	6
1526	ATOM	CB VAL A 186	41.807	20.506	43.735	1.00	8.32	6
1527	ATOM	CG VAL A 186	41.196	21.617	44.616	1.00	7.05	6
1528	ATOM	CD2 VAL A 186	43.173	20.110	44.308	1.00	5.20	6
1529	ATOM	C VAL A 186	41.364	18.291	42.578	1.00	8.42	6
1530	ATOM	O VAL A 186	41.505	17.111	42.956	1.00	8.25	8
1531	ATOM	H SER A 187	41.735	18.666	41.367	1.00	8.40	7
1532	ATOM	CA SER A 187	42.313	17.723	40.445	1.00	8.96	6
1533	ATOM	CB SER A 187	42.664	18.422	39.113	1.00	8.95	6
1534	ATOM	CG SER A 187	43.472	17.537	38.328	1.00	8.65	8
1535	ATOM	CD SER A 187	43.603	17.153	41.060	1.00	9.46	6
1536	ATOM	O SER A 187	44.375	17.887	41.684	1.00	9.28	8
1537	ATOM	H SER A 188	43.908	15.846	40.823	1.00	9.77	7
1538	ATOM	CA SER A 188	45.109	15.208	41.353	1.00	9.72	6
1539	ATOM	CB SER A 188	44.906	13.770	41.859	1.00	10.83	6
1540	ATOM	OG SER A 188	46.547	12.983	40.714	1.00	12.11	8
1541	ATOM	C SER A 188	46.215	15.213	40.288	1.00	9.72	6
1542	ATOM	O SER A 188	47.239	14.540	40.529	1.00	9.62	8
1543	ATOM	N GLU A 189	46.009	15.968	39.192	1.00	9.48	7
1544	ATOM	CA GLU A 189	47.091	16.143	38.252	1.00	9.58	6
1545	ATOM	CB GLU A 189	46.761	17.025	37.029	1.00	12.65	6
1546	ATOM	CG GLU A 189	45.655	16.361	36.202	1.00	14.93	6
1547	ATOM	CD GLU A 189	44.958	17.419	35.359	1.00	16.59	6
1548	ATOM	OE1 GLU A 189	44.060	18.118	35.668	1.00	16.06	8
1549	ATOM	OE2 GLU A 189	45.364	17.496	34.187	1.00	19.90	8
1550	ATOM	C GLU A 189	47.948	17.852	39.783	1.00	9.35	8
1551	ATOM	O GLU A 189	49.447	16.512	38.785	1.00	9.02	7
1552	ATOM	N ASN A 190	50.591	17.137	39.437	1.00	8.98	6
1553	ATOM	CA ASN A 190	50.708	18.629	39.139	1.00	11.63	6
1554	ATOM	CB ASN A 190	50.842	19.067	37.714	1.00	13.22	6
1555	ATOM	CG ASN A 190	51.553	18.489	36.913	1.00	13.96	8
1556	ATOM	CD1 ASN A 190	50.145	20.093	37.234	1.00	14.84	7
1557	ATOM	CD2 ASN A 190	50.548	16.928	40.959	1.00	8.84	6
1558	ATOM	C ASN A 190	51.020	17.773	41.750	1.00	9.06	8
1559	ATOM	O ASN A 190	49.949	15.854	41.439	1.00	8.36	7
1560	ATOM	N GLY A 191	49.772	15.467	42.809	1.00	7.95	6
1561	ATOM	CA GLY A 191	48.597	16.148	43.430	1.00	7.74	6
1562	ATOM	C GLY A 191	47.747	15.586	44.065	1.00	7.89	8
1563	ATOM	O GLY A 191	48.537	17.450	43.284	1.00	7.66	7
1564	ATOM	N ASN A 192	47.472	18.353	43.732	1.00	7.21	6
1565	ATOM	CA ASN A 192	47.596	18.649	45.227	1.00	8.14	6
1566	ATOM	CB ASN A 192	46.628	19.665	45.785	1.00	7.93	6
1567	ATOM	CG ASN A 192	46.584	20.794	45.287	1.00	8.55	8
1568	ATOM	CD1 ASN A 192	45.839	19.388	46.805	1.00	7.17	7
1569	ATOM	CD2 ASN A 192	47.572	19.615	42.863	1.00	6.90	6
1570	ATOM	C ASN A 192	48.574	20.328	42.910	1.00	6.69	8
1571	ATOM	O ASN A 192	46.517	19.881	42.099	1.00	6.77	7
1572	ATOM	N TYR A 193	46.405	20.986	41.210	1.00	7.00	6
1573	ATOM	CA TYR A 193	45.725	20.535	39.867	1.00	7.52	6
1574	ATOM	CB TYR A 193	46.348	21.143	38.659	1.00	8.30	6
1575	ATOM	CG TYR A 193	46.218	20.596	37.385	1.00	8.97	6
1576	ATOM	CD1 TYR A 193	46.841	21.202	36.283	1.00	9.17	6
1577	ATOM	CD2 TYR A 193	47.096	22.301	38.738	1.00	8.68	6
1578	ATOM	CE2 TYR A 193	47.695	22.928	37.673	1.00	9.08	6
1579	ATOM	CE3 TYR A 193	47.564	22.343	36.424	1.00	9.29	6
1580	ATOM	CZ TYR A 193	48.177	22.966	35.361	1.00	9.62	8
1581	ATOM	OH TYR A 193	45.036	22.979	41.061	1.00	6.92	6
1582	ATOM	O TYR A 193	45.646	22.201	41.778	1.00	6.78	8
1583	ATOM	C TYR A 193	45.662	22.448	43.066	1.00	6.98	7
1584	ATOM	N ASP A 194	45.102	23.587	43.773	1.00	6.81	6
1585	ATOM	CA ASP A 194	45.338	23.579	45.279	1.00	7.26	6
1586	ATOM	CB ASP A 194	44.586	24.609	46.082	1.00	8.65	6
1587	ATOM	CG ASP A 194	43.590	25.127	45.523	1.00	9.18	8
1588	ATOM	CD1 ASP A 194	44.730	24.922	47.280	1.00	8.67	8
1589	ATOM	CD2 ASP A 194	45.815	24.809	43.156	1.00	6.63	6
1590	ATOM	C ASP A 194						

ATOM	1591	O	ASP A 194	45.143	25.681	42.616	1.00	6.42	8
ATOM	1592	N	YR A 195	47.129	26.919	43.145	1.00	6.43	7
ATOM	1593	CA	YR A 195	47.781	26.059	42.596	1.00	6.19	6
ATOM	1594	CG	YR A 195	49.261	26.101	43.153	1.00	5.52	6
ATOM	1595	CB	YR A 195	49.722	27.472	42.821	1.00	5.15	6
ATOM	1596	CD1	YR A 195	49.314	28.569	43.582	1.00	5.28	6
ATOM	1597	CE1	YR A 195	49.676	29.862	43.186	1.00	5.27	6
ATOM	1598	CD2	YR A 195	50.456	27.686	41.665	1.00	5.05	6
ATOM	1599	CE2	YR A 195	50.809	28.972	41.246	1.00	5.04	6
ATOM	1600	CZ	YR A 195	50.386	30.053	42.030	1.00	5.27	6
ATOM	1601	OH	YR A 195	50.742	31.310	41.636	1.00	5.27	8
ATOM	1602	C	YR A 195	47.730	26.123	41.082	1.00	6.73	6
ATOM	1603	O	YR A 195	48.128	25.186	40.392	1.00	6.74	8
ATOM	1604	N	LEU A 196	47.329	27.323	40.580	1.00	7.17	7
ATOM	1605	CA	LEU A 196	47.366	27.572	39.148	1.00	7.71	6
ATOM	1606	CB	LEU A 196	45.962	27.721	38.510	1.00	6.89	6
ATOM	1607	CG	LEU A 196	45.988	28.100	37.020	1.00	8.29	6
ATOM	1608	CD1	LEU A 196	46.520	26.975	36.126	1.00	6.67	6
ATOM	1609	CD2	LEU A 196	44.578	28.516	36.621	1.00	7.69	6
ATOM	1610	C	LEU A 196	48.181	28.816	38.807	1.00	7.86	6
ATOM	1611	O	LEU A 196	49.162	28.671	38.073	1.00	7.98	8
ATOM	1612	N	MET A 197	47.861	29.990	39.319	1.00	7.94	7
ATOM	1613	CA	MET A 197	48.577	31.228	39.029	1.00	8.00	6
ATOM	1614	CB	MET A 197	46.230	31.699	37.613	1.00	11.16	6
ATOM	1615	CG	MET A 197	46.758	32.064	37.445	1.00	15.62	6
ATOM	1616	SD	MET A 197	46.223	32.419	35.732	1.00	22.83	16
ATOM	1617	CE	MET A 197	47.695	33.237	35.117	1.00	21.60	6
ATOM	1618	C	MET A 197	48.157	32.310	40.032	1.00	7.71	6
ATOM	1619	O	MET A 197	47.200	32.162	40.792	1.00	7.22	8
ATOM	1620	N	YR A 198	48.875	33.421	39.997	1.00	7.95	7
ATOM	1621	CA	YR A 198	48.725	34.595	40.649	1.00	8.22	6
ATOM	1622	CB	YR A 198	47.512	35.420	40.476	1.00	9.23	6
ATOM	1623	CG	YR A 198	47.601	35.991	39.081	1.00	10.99	6
ATOM	1624	CD1	YR A 198	46.600	35.690	38.145	1.00	11.90	6
ATOM	1625	CE1	YR A 198	46.655	36.230	36.875	1.00	12.83	6
ATOM	1626	CD2	YR A 198	48.664	36.817	38.741	1.00	11.91	6
ATOM	1627	CE2	YR A 198	48.745	37.364	37.443	1.00	12.82	6
ATOM	1628	CZ	YR A 198	47.741	37.045	36.538	1.00	13.43	6
ATOM	1629	OH	YR A 198	47.797	37.589	35.261	1.00	14.37	8
ATOM	1630	C	YR A 198	48.629	34.167	42.312	1.00	7.86	6
ATOM	1631	O	YR A 198	49.362	33.257	42.693	1.00	7.88	8
ATOM	1632	N	ALA A 199	47.769	34.787	43.117	1.00	7.31	7
ATOM	1633	CA	ALA A 199	47.563	34.481	44.537	1.00	6.22	6
ATOM	1634	CB	ALA A 199	47.321	35.747	45.359	1.00	6.48	6
ATOM	1635	C	ALA A 199	46.389	33.523	44.687	1.00	5.38	6
ATOM	1636	O	ALA A 199	45.255	33.918	44.370	1.00	5.00	8
ATOM	1637	N	ASP A 200	46.702	32.319	45.148	1.00	5.09	7
ATOM	1638	CA	ASP A 200	45.748	31.224	45.295	1.00	5.00	6
ATOM	1639	CB	ASP A 200	46.567	29.901	45.278	1.00	5.25	6
ATOM	1640	CG	ASP A 200	45.495	28.798	45.141	1.00	6.80	6
ATOM	1641	CD1	ASP A 200	44.912	28.830	44.024	1.00	6.41	8
ATOM	1642	CD2	ASP A 200	45.139	27.965	46.011	1.00	6.48	8
ATOM	1643	C	ASP A 200	44.879	31.313	46.526	1.00	5.00	6
ATOM	1644	O	ASP A 200	45.308	31.320	47.681	1.00	5.31	8
ATOM	1645	N	VAL A 201	43.567	31.445	46.359	1.00	5.00	7
ATOM	1646	CA	VAL A 201	42.610	31.603	47.446	1.00	5.00	6
ATOM	1647	CB	VAL A 201	41.215	31.999	46.911	1.00	5.00	6
ATOM	1648	CG1	VAL A 201	40.249	32.082	48.071	1.00	5.00	6
ATOM	1649	CG2	VAL A 201	41.205	33.336	46.136	1.00	5.00	6
ATOM	1650	C	VAL A 201	42.542	30.306	48.243	1.00	5.00	6
ATOM	1651	O	VAL A 201	42.387	29.199	47.732	1.00	5.00	8
ATOM	1652	N	ASP A 202	42.605	30.491	49.571	1.00	5.00	7
ATOM	1653	CA	ASP A 202	42.519	29.430	50.556	1.00	5.00	6
ATOM	1654	CB	ASP A 202	43.337	29.878	51.801	1.00	5.82	6
ATOM	1655	CG	ASP A 202	43.437	28.834	52.876	1.00	6.39	6
ATOM	1656	CD1	ASP A 202	42.805	27.761	52.605	1.00	5.70	8
ATOM	1657	CD2	ASP A 202	44.017	28.814	53.965	1.00	6.27	8
ATOM	1658	C	ASP A 202	41.060	29.141	50.949	1.00	5.00	6
ATOM	1659	O	ASP A 202	40.518	29.810	51.838	1.00	5.00	8
ATOM	1660	N	YR A 203	40.418	28.138	50.330	1.00	5.00	7
ATOM	1661	CA	YR A 203	39.019	27.825	50.636	1.00	5.09	6
ATOM	1662	CB	YR A 203	38.234	27.239	49.448	1.00	5.00	6
ATOM	1663	CG	YR A 203	38.008	28.366	48.426	1.00	5.00	6
ATOM	1664	CD1	YR A 203	38.653	28.457	47.236	1.00	5.00	6
ATOM	1665	CE1	YR A 203	38.449	29.510	46.379	1.00	5.00	6
ATOM	1666	CD2	YR A 203	37.124	29.393	48.827	1.00	5.05	6
ATOM	1667	CE2	YR A 203	36.914	30.493	47.963	1.00	5.07	6
ATOM	1668	CZ	YR A 203	37.577	30.536	46.763	1.00	5.13	6
ATOM	1669	OH	YR A 203	37.355	31.607	45.918	1.00	5.71	8
ATOM	1670	C	YR A 203	38.899	26.963	51.897	1.00	5.73	6
ATOM	1671	O	YR A 203	37.783	26.505	52.205	1.00	5.91	8
ATOM	1672	N	ASP A 204	39.942	26.807	52.703	1.00	6.06	7
ATOM	1673	CA	ASP A 204	39.883	26.202	54.010	1.00	6.93	6
ATOM	1674	CB	ASP A 204	41.108	25.454	54.543	1.00	7.71	6
ATOM	1675	CG	ASP A 204	41.389	24.192	53.738	1.00	9.87	6
ATOM	1676	CD1	ASP A 204	40.413	23.443	53.469	1.00	11.60	8
ATOM	1677	CD2	ASP A 204	42.553	23.870	53.354	1.00	10.31	8
ATOM	1678	C	ASP A 204	39.632	27.395	55.016	1.00	7.25	6
ATOM	1679	O	ASP A 204	39.231	27.113	56.154	1.00	7.19	8
ATOM	1680	N	HIS A 205	39.838	28.671	54.654	1.00	7.01	7
ATOM	1681	CA	HIS A 205	39.660	29.773	55.659	1.00	7.00	6
ATOM	1682	CB	HIS A 205	40.519	30.961	55.174	1.00	5.97	6
ATOM	1683	CG	HIS A 205	40.566	32.025	56.220	1.00	7.15	6
ATOM	1684	CD2	HIS A 205	39.590	32.773	56.780	1.00	5.16	6
ATOM	1685	MD1	HIS A 205	41.751	32.331	56.910	1.00	8.31	7
ATOM	1686	CE1	HIS A 205	41.525	33.260	57.828	1.00	6.29	6
ATOM	1687	ME2	HIS A 205	40.214	33.513	57.752	1.00	8.24	7
ATOM	1688	C	HIS A 205	38.199	30.050	55.824	1.00	7.15	6
ATOM	1689	O	HIS A 205	37.511	30.307	54.825	1.00	7.72	8
ATOM	1690	N	PRO A 206	37.579	29.986	56.988	1.00	6.98	7
ATOM	1691	CD	PRO A 206	38.242	29.637	58.262	1.00	6.83	6
ATOM	1692	CA	PRO A 206	36.134	30.164	57.160	1.00	6.77	6
ATOM	1693	CB	PRO A 206	35.776	29.837	58.641	1.00	6.82	6
ATOM	1694	CG	PRO A 206	37.146	30.071	59.263	1.00	6.98	6
ATOM	1695	C	PRO A 206	35.653	31.549	56.764	1.00	6.49	6
ATOM	1696	O	PRO A 206	34.527	31.608	56.238	1.00	6.33	8

ATOM	1697	N	ASP	A	207	36.466	32.591	56.971	1.00	6.12	7	ATOM	1750	CA	LYS	A	214	28.061	36.774	50.337	1.00	7.39	6
ATOM	1698	CA	ASP	A	207	36.056	33.949	56.613	1.00	6.05	6	ATOM	1751	CB	LYS	A	214	28.638	37.530	51.539	1.00	11.90	6
ATOM	1699	CB	ASP	A	207	36.954	35.059	57.168	1.00	6.37	6	ATOM	1752	CD	LYS	A	214	28.423	39.011	51.741	1.00	17.64	6
ATOM	1700	CG	ASP	A	207	36.964	35.075	58.705	1.00	6.87	6	ATOM	1753	CD	LYS	A	214	29.354	39.548	52.915	1.00	22.01	6
ATOM	1701	CD1	ASP	A	207	36.208	34.392	59.396	1.00	6.00	8	ATOM	1754	CE	LYS	A	214	29.770	41.017	52.697	1.00	24.62	6
ATOM	1702	CD2	ASP	A	207	37.779	35.836	59.261	1.00	7.95	8	ATOM	1755	WZ	LYS	A	214	31.138	41.472	53.171	1.00	24.85	7
ATOM	1703	C	ASP	A	207	36.033	34.139	55.096	1.00	6.17	6	ATOM	1756	C	LYS	A	214	28.290	37.533	49.021	1.00	7.07	6
ATOM	1704	O	ASP	A	207	35.225	34.906	54.573	1.00	5.78	8	ATOM	1757	O	LYS	A	214	27.317	38.174	48.561	1.00	7.02	8
ATOM	1705	N	VAL	A	208	36.985	33.441	54.427	1.00	6.47	7	ATOM	1758	N	TRP	A	215	29.481	37.502	48.430	1.00	6.68	7
ATOM	1706	CA	VAL	A	208	37.054	33.472	52.973	1.00	6.58	6	ATOM	1759	CA	TRP	A	215	29.726	38.173	47.140	1.00	6.58	6
ATOM	1707	CB	VAL	A	208	38.353	32.859	52.465	1.00	7.47	6	ATOM	1760	CB	TRP	A	215	31.216	38.139	46.715	1.00	5.00	6
ATOM	1708	CG1	VAL	A	208	38.292	32.594	50.949	1.00	7.06	6	ATOM	1761	CG	TRP	A	215	31.353	38.622	45.281	1.00	5.00	6
ATOM	1709	CG2	VAL	A	208	39.526	33.788	52.805	1.00	6.71	6	ATOM	1762	CG2	TRP	A	215	31.418	37.741	44.122	1.00	5.00	6
ATOM	1710	C	VAL	A	208	35.795	32.784	52.426	1.00	6.90	6	ATOM	1763	CE2	TRP	A	215	31.427	38.544	43.003	1.00	5.00	6
ATOM	1711	O	VAL	A	208	35.103	33.349	51.530	1.00	6.93	7	ATOM	1764	CE3	TRP	A	215	31.455	36.349	43.980	1.00	5.00	6
ATOM	1712	N	VAL	A	209	35.436	31.598	52.923	1.00	6.93	8	ATOM	1765	CD1	TRP	A	215	31.355	39.909	44.808	1.00	5.00	6
ATOM	1713	CA	VAL	A	209	34.257	30.881	52.457	1.00	7.00	6	ATOM	1766	NE1	TRP	A	215	31.418	39.874	43.430	1.00	5.00	7
ATOM	1714	CB	VAL	A	209	34.140	29.527	53.170	1.00	5.34	6	ATOM	1767	CG2	TRP	A	215	31.507	38.008	41.720	1.00	5.00	6
ATOM	1715	CG1	VAL	A	209	32.865	28.784	52.814	1.00	5.00	6	ATOM	1768	CG3	TRP	A	215	31.494	35.789	42.707	1.00	5.18	6
ATOM	1716	CG2	VAL	A	209	35.346	28.638	52.878	1.00	5.00	6	ATOM	1769	CH2	TRP	A	215	31.534	36.649	41.559	1.00	5.00	6
ATOM	1717	C	VAL	A	209	32.996	31.743	52.652	1.00	7.32	6	ATOM	1770	O	TRP	A	215	28.836	37.573	46.045	1.00	6.80	6
ATOM	1718	O	VAL	A	209	32.199	31.882	51.686	1.00	7.35	8	ATOM	1771	O	TRP	A	215	28.222	38.231	45.223	1.00	6.73	8
ATOM	1719	N	ALA	A	210	32.798	32.341	53.838	1.00	7.34	7	ATOM	1772	N	GLY	A	216	28.714	36.209	46.000	1.00	7.00	7
ATOM	1720	CA	ALA	A	210	31.623	33.165	54.102	1.00	7.52	6	ATOM	1773	CA	GLY	A	216	27.936	35.541	45.004	1.00	7.12	6
ATOM	1721	CB	ALA	A	210	31.558	33.591	53.584	1.00	7.62	6	ATOM	1774	C	GLY	A	216	26.482	35.990	44.999	1.00	7.24	6
ATOM	1722	C	ALA	A	210	31.490	34.416	53.261	1.00	7.58	6	ATOM	1775	O	GLY	A	216	25.868	36.132	43.918	1.00	6.99	8
ATOM	1723	O	ALA	A	210	30.401	34.806	52.803	1.00	7.48	8	ATOM	1776	N	ILE	A	217	25.955	36.136	46.205	1.00	7.41	7
ATOM	1724	N	GLU	A	211	32.614	35.095	53.060	1.00	7.67	7	ATOM	1777	CA	ILE	A	217	24.531	36.546	46.325	1.00	7.50	6
ATOM	1725	CA	GLU	A	211	32.662	36.296	52.216	1.00	7.90	6	ATOM	1778	CB	ILE	A	217	24.011	36.340	47.777	1.00	8.38	6
ATOM	1726	CB	GLU	A	211	34.061	36.946	52.363	1.00	9.96	6	ATOM	1779	CG2	ILE	A	217	22.627	36.981	48.057	1.00	6.66	6
ATOM	1727	CG	GLU	A	211	34.267	38.168	51.517	1.00	13.89	6	ATOM	1780	CG1	ILE	A	217	23.923	34.851	48.131	1.00	7.56	6
ATOM	1728	CD	GLU	A	211	33.197	39.270	51.640	1.00	16.28	6	ATOM	1781	CD1	ILE	A	217	24.065	34.682	49.629	1.00	7.44	6
ATOM	1729	OE1	GLU	A	211	32.845	39.772	50.515	1.00	18.47	8	ATOM	1782	C	ILE	A	217	24.406	37.971	45.846	1.00	7.47	6
ATOM	1730	OE2	GLU	A	211	32.747	39.610	52.771	1.00	13.34	8	ATOM	1783	O	ILE	A	217	23.541	38.350	45.092	1.00	7.49	8
ATOM	1731	C	GLU	A	211	32.384	36.053	50.721	1.00	7.61	6	ATOM	1784	N	TRP	A	218	25.329	38.844	46.222	1.00	7.72	7
ATOM	1732	O	GLU	A	211	31.758	36.890	50.040	1.00	7.56	8	ATOM	1785	CA	TRP	A	218	25.354	40.252	45.814	1.00	7.84	6
ATOM	1733	N	THR	A	212	32.907	34.960	50.184	1.00	7.17	7	ATOM	1786	CB	TRP	A	218	26.556	40.953	46.464	1.00	7.78	6
ATOM	1734	CA	THR	A	212	32.727	34.572	48.781	1.00	6.96	6	ATOM	1787	CG	TRP	A	218	26.778	42.365	45.975	1.00	8.77	6
ATOM	1735	CB	THR	A	212	33.705	33.444	48.413	1.00	8.17	6	ATOM	1788	CG2	TRP	A	218	27.638	42.809	44.926	1.00	8.24	6
ATOM	1736	OG1	THR	A	212	35.056	33.934	48.636	1.00	9.40	8	ATOM	1789	CG2	TRP	A	218	27.466	44.221	44.817	1.00	9.24	6
ATOM	1737	CG2	THR	A	212	33.660	33.139	48.939	1.00	7.69	6	ATOM	1790	CE3	TRP	A	218	28.514	42.168	44.041	1.00	7.35	6
ATOM	1738	C	THR	A	212	31.276	34.155	48.554	1.00	6.87	6	ATOM	1791	CD1	TRP	A	218	26.112	43.473	46.439	1.00	9.49	6
ATOM	1739	O	THR	A	212	30.724	34.456	47.522	1.00	6.69	8	ATOM	1792	ME1	TRP	A	218	26.535	44.589	45.737	1.00	8.69	6
ATOM	1740	N	LYS	A	213	30.604	33.516	49.527	1.00	6.92	7	ATOM	1793	CG2	TRP	A	218	28.169	45.022	43.903	1.00	7.92	6
ATOM	1741	CA	LYS	A	213	29.168	33.214	49.424	1.00	7.14	6	ATOM	1794	CG3	TRP	A	218	29.215	42.962	43.149	1.00	8.47	6
ATOM	1742	CB	LYS	A	213	28.634	32.331	50.553	1.00	6.97	6	ATOM	1795	CH2	TRP	A	218	29.058	44.371	43.069	1.00	7.81	6
ATOM	1743	CG	LYS	A	213	29.076	30.863	50.321	1.00	9.06	6	ATOM	1796	C	TRP	A	218	25.395	40.438	44.301	1.00	7.56	8
ATOM	1744	CD	LYS	A	213	28.605	30.065	51.592	1.00	9.86	6	ATOM	1797	O	TRP	A	218	26.708	41.250	43.686	1.00	8.18	7
ATOM	1745	CE	LYS	A	213	29.312	28.701	51.442	1.00	10.33	6	ATOM	1798	N	TYR	A	219	26.300	39.722	43.653	1.00	8.37	6
ATOM	1746	NZ	LYS	A	213	28.914	27.848	52.609	1.00	11.44	7	ATOM	1799	CA	TYR	A	219	26.537	39.709	42.203	1.00	8.61	6
ATOM	1747	C	LYS	A	213	28.352	34.524	49.417	1.00	7.15	6	ATOM	1800	CG	TYR	A	219	27.703	38.789	41.955	1.00	9.11	6
ATOM	1748	O	LYS	A	213	27.462	34.755	48.620	1.00	6.94	8	ATOM	1801	CG	TYR	A	219	28.243	38.670	40.554	1.00	9.11	6
ATOM	1749	N	LYS	A	214	28.687	35.476	50.279	1.00	7.01	7	ATOM	1802	CD1	TYR	A	219	28.615	39.784	39.810	1.00	9.59	6

ATOM	1803	CE1 TYR A 219	29.180	39.619	38.561	1.00	9.96	6	ATOM	1856	CB ASP A 226	19.357	33.821	34.254	1.00	7.73	6
ATOM	1804	CD2 TYR A 219	28.416	37.404	40.008	1.00	9.35	6	ATOM	1857	CG ASP A 226	18.559	35.071	33.990	1.00	7.95	6
ATOM	1805	CE2 TYR A 219	28.959	37.265	38.760	1.00	9.78	6	ATOM	1858	CD1 ASP A 226	17.512	35.272	33.681	1.00	10.67	8
ATOM	1806	CF2 TYR A 219	29.346	38.361	38.021	1.00	10.19	6	ATOM	1859	CD2 ASP A 226	18.962	35.869	33.172	1.00	7.61	8
ATOM	1807	OH TYR A 219	29.899	38.187	36.757	1.00	11.08	8	ATOM	1860	C ASP A 226	20.796	32.668	35.806	1.00	7.95	6
ATOM	1808	C TYR A 219	25.279	39.259	41.467	1.00	8.69	6	ATOM	1861	O ASP A 226	20.213	31.578	35.837	1.00	8.41	8
ATOM	1809	O TYR A 219	24.836	39.946	40.527	1.00	8.37	8	ATOM	1862	N GLY A 227	22.107	32.836	35.852	1.00	7.65	7
ATOM	1810	N ALA A 220	24.676	38.131	41.869	1.00	9.13	7	ATOM	1863	CA GLY A 227	22.992	31.679	35.946	1.00	7.46	6
ATOM	1811	CB ALA A 220	23.427	37.644	41.267	1.00	9.77	6	ATOM	1864	C GLY A 227	24.471	32.049	35.990	1.00	7.30	6
ATOM	1812	CA ALA A 220	22.899	36.364	41.981	1.00	8.61	6	ATOM	1865	O GLY A 228	24.880	33.197	36.042	1.00	6.95	8
ATOM	1813	C ALA A 220	22.315	38.685	41.321	1.00	10.07	6	ATOM	1866	N PHE A 228	25.294	30.990	36.029	1.00	7.33	7
ATOM	1814	O ALA A 220	21.536	38.887	40.377	1.00	10.05	8	ATOM	1867	CA PHE A 228	26.742	31.170	36.146	1.00	7.35	6
ATOM	1815	N ASN A 221	22.192	39.338	42.473	1.00	10.39	7	ATOM	1868	CG PHE A 228	27.220	30.898	37.558	1.00	6.74	6
ATOM	1816	CA ASN A 221	21.200	40.374	42.757	1.00	10.66	6	ATOM	1869	CG PHE A 228	26.640	31.708	38.672	1.00	9.48	6
ATOM	1817	CB ASN A 221	21.013	40.698	44.262	1.00	13.90	6	ATOM	1870	CD1 PHE A 228	25.930	31.082	39.700	1.00	9.82	6
ATOM	1818	CG ASN A 221	20.192	39.343	44.855	1.00	18.18	6	ATOM	1871	CD2 PHE A 228	26.800	33.097	38.702	1.00	8.78	6
ATOM	1819	CD1 ASN A 221	19.371	38.952	44.227	1.00	19.46	8	ATOM	1872	CE1 PHE A 228	25.415	31.869	40.731	1.00	10.75	6
ATOM	1820	ND2 ASN A 221	20.681	39.263	46.125	1.00	19.86	7	ATOM	1873	CE2 PHE A 228	26.277	33.860	39.746	1.00	9.42	6
ATOM	1821	C ASN A 221	21.524	41.717	42.136	1.00	10.51	6	ATOM	1874	CZ PHE A 228	25.590	33.241	40.786	1.00	9.64	6
ATOM	1822	O ASN A 221	22.794	42.125	42.163	1.00	10.40	8	ATOM	1875	C PHE A 228	27.603	30.229	35.304	1.00	7.29	6
ATOM	1823	N GLU A 222	23.160	43.432	41.552	1.00	10.18	6	ATOM	1876	O PHE A 228	27.245	29.086	34.995	1.00	7.76	8
ATOM	1824	CA GLU A 222	25.013	45.244	41.469	1.00	12.96	6	ATOM	1877	N ARG A 229	28.791	30.675	34.978	1.00	6.86	7
ATOM	1825	CG GLU A 222	24.621	43.807	41.791	1.00	11.08	6	ATOM	1878	CA ARG A 229	29.818	29.927	34.305	1.00	6.75	6
ATOM	1826	CG GLU A 222	25.412	46.203	42.696	1.00	15.13	6	ATOM	1879	CB ARG A 229	30.172	30.439	32.885	1.00	6.68	6
ATOM	1827	CD GLU A 222	23.947	45.777	43.576	1.00	15.79	8	ATOM	1880	CG ARG A 229	31.309	29.551	32.327	1.00	5.59	6
ATOM	1828	OE1 GLU A 222	24.381	47.432	42.576	1.00	16.17	8	ATOM	1881	CD ARG A 229	32.846	30.283	32.584	1.00	7.61	7
ATOM	1829	OE2 GLU A 222	22.903	43.428	40.052	1.00	9.82	6	ATOM	1882	NE ARG A 229	33.701	29.623	31.828	1.00	7.61	7
ATOM	1830	C GLU A 222	22.470	44.444	39.507	1.00	9.72	8	ATOM	1883	CZ ARG A 229	34.985	29.905	31.872	1.00	8.29	6
ATOM	1831	O GLU A 222	23.227	42.343	39.348	1.00	9.48	7	ATOM	1884	HH2 ARG A 229	35.833	29.189	31.139	1.00	7.90	7
ATOM	1832	N LEU A 223	23.009	42.319	37.909	1.00	9.43	6	ATOM	1885	HH1 ARG A 229	35.388	30.913	32.626	1.00	7.66	7
ATOM	1833	CA LEU A 223	24.300	41.715	37.281	1.00	7.13	6	ATOM	1886	C ARG A 229	30.998	29.916	35.323	1.00	6.49	6
ATOM	1834	CB LEU A 223	25.595	42.503	37.476	1.00	5.72	6	ATOM	1887	O ARG A 229	31.518	30.980	35.697	1.00	6.39	8
ATOM	1835	CG LEU A 223	26.752	41.715	36.835	1.00	5.00	6	ATOM	1888	N ILE A 230	31.427	28.711	35.760	1.00	6.19	7
ATOM	1836	CD1 LEU A 223	25.470	43.808	36.880	1.00	5.20	6	ATOM	1889	CA ILE A 230	32.530	28.667	36.752	1.00	5.82	6
ATOM	1837	CD2 LEU A 223	21.794	41.550	37.456	1.00	9.44	6	ATOM	1890	CB ILE A 230	32.239	27.598	37.860	1.00	6.87	6
ATOM	1838	C LEU A 223	21.561	41.335	36.280	1.00	9.37	8	ATOM	1891	CG2 ILE A 230	33.534	27.325	38.636	1.00	5.00	6
ATOM	1839	O LEU A 223	20.953	40.998	38.286	1.00	9.74	7	ATOM	1892	CG1 ILE A 230	31.001	28.126	38.637	1.00	6.60	6
ATOM	1840	N SER A 224	19.825	40.156	37.925	1.00	10.06	6	ATOM	1893	CD1 ILE A 230	30.470	27.073	39.606	1.00	11.75	6
ATOM	1841	CA SER A 224	18.660	40.832	37.156	1.00	19.93	8	ATOM	1894	C ILE A 230	33.907	28.409	36.148	1.00	5.56	6
ATOM	1842	CG SER A 224	18.251	41.991	37.901	1.00	9.76	6	ATOM	1895	O ILE A 230	34.225	27.368	35.555	1.00	5.42	8
ATOM	1843	OG SER A 224	20.293	38.979	37.047	1.00	9.76	6	ATOM	1896	N ASP A 231	34.758	29.428	36.246	1.00	5.02	7
ATOM	1844	C SER A 224	19.648	38.752	36.004	1.00	9.20	7	ATOM	1897	CA ASP A 231	36.086	29.322	35.714	1.00	5.00	6
ATOM	1845	O SER A 224	21.340	38.248	37.445	1.00	9.74	8	ATOM	1898	CG ASP A 231	36.693	30.766	35.684	1.00	5.00	6
ATOM	1846	N LEU A 225	21.770	37.113	36.651	1.00	8.94	6	ATOM	1899	CG ASP A 231	38.078	30.857	35.062	1.00	5.00	6
ATOM	1847	CA LEU A 225	23.164	36.688	37.088	1.00	10.36	6	ATOM	1900	CD1 ASP A 231	38.156	30.584	33.864	1.00	5.00	8
ATOM	1848	CB LEU A 225	24.297	37.738	36.958	1.00	11.62	6	ATOM	1901	CD2 ASP A 231	39.013	31.237	35.828	1.00	5.00	8
ATOM	1849	CG LEU A 225	25.552	37.149	37.597	1.00	10.68	6	ATOM	1902	C ASP A 231	37.016	28.427	36.518	1.00	5.00	6
ATOM	1850	CD1 LEU A 225	24.524	38.163	35.508	1.00	10.53	6	ATOM	1903	O ASP A 231	36.987	28.462	37.750	1.00	5.00	8
ATOM	1851	CD2 LEU A 225	20.793	35.945	36.627	1.00	8.77	6	ATOM	1904	N ALA A 232	37.861	27.681	35.819	1.00	5.00	7
ATOM	1852	C LEU A 225	20.084	35.785	37.796	1.00	8.46	8	ATOM	1905	CA ALA A 232	38.889	26.846	36.430	1.00	5.00	6
ATOM	1853	O LEU A 225	20.734	35.084	35.804	1.00	8.55	7	ATOM	1906	CB ALA A 232	39.930	27.869	36.945	1.00	6.65	6
ATOM	1854	N ASP A 226	19.950	33.911	35.674	1.00	7.98	6	ATOM	1907	C ALA A 232	38.515	25.954	37.593	1.00	5.00	6
ATOM	1855	CA ASP A 226							ATOM	1908	O ALA A 232	39.189	25.916	38.626	1.00	5.00	8

ATOM	1909	N	ALA A 233	37.399	25.223	37.414	1.00	5.00	7	7	ATOM	1963	CA	SER A 239	32.706	20.656	48.065	1.00	7.57	6	6
ATOM	1910	CA	ALA A 233	36.848	24.420	38.465	1.00	5.45	6	6	ATOM	1964	OG	SER A 239	32.940	19.984	49.417	1.00	7.79	6	6
ATOM	1911	CB	ALA A 233	35.529	23.866	37.899	1.00	6.05	6	6	ATOM	1965	O	SER A 239	34.169	22.443	49.919	1.00	10.61	8	8
ATOM	1912	C	ALA A 233	37.755	23.310	38.952	1.00	6.00	6	6	ATOM	1966	O	SER A 239	32.410	22.159	48.249	1.00	7.33	6	6
ATOM	1913	O	ALA A 233	37.565	22.963	40.144	1.00	6.16	8	8	ATOM	1967	N	PHE A 240	31.237	22.448	48.454	1.00	7.20	6	6
ATOM	1914	N	LYS A 234	38.683	22.764	38.169	1.00	5.81	7	7	ATOM	1968	CA	PHE A 240	33.380	23.066	48.168	1.00	7.19	7	7
ATOM	1915	CA	LYS A 234	39.508	21.670	38.618	1.00	6.08	6	6	ATOM	1969	CB	PHE A 240	33.073	24.471	48.275	1.00	7.28	6	6
ATOM	1916	CB	LYS A 234	40.171	20.929	37.485	1.00	5.76	6	6	ATOM	1970	CG	PHE A 240	34.332	25.325	48.382	1.00	7.42	6	6
ATOM	1917	CG	LYS A 234	41.275	21.620	36.704	1.00	6.41	6	6	ATOM	1971	CG	PHE A 240	34.049	26.801	48.123	1.00	7.00	6	6
ATOM	1918	CD	LYS A 234	41.843	20.613	35.671	1.00	7.10	6	6	ATOM	1972	CD1	PHE A 240	33.390	27.560	49.085	1.00	6.31	6	6
ATOM	1919	CE	LYS A 234	43.116	21.208	34.994	1.00	5.42	6	6	ATOM	1973	CD2	PHE A 240	34.413	27.352	46.911	1.00	6.51	6	6
ATOM	1920	HZ	LYS A 234	43.541	20.287	33.901	1.00	5.00	7	7	ATOM	1974	CE1	PHE A 240	33.091	28.886	48.775	1.00	7.11	6	6
ATOM	1921	C	LYS A 234	40.530	22.145	39.648	1.00	6.60	6	6	ATOM	1975	CE2	PHE A 240	34.116	28.674	46.615	1.00	5.97	6	6
ATOM	1922	O	LYS A 234	41.110	21.289	40.336	1.00	6.53	8	8	ATOM	1976	C	PHE A 240	33.479	29.440	47.555	1.00	5.18	6	6
ATOM	1923	N	HIS A 235	40.709	23.486	39.781	1.00	6.73	7	7	ATOM	1977	O	PHE A 240	32.259	24.900	47.044	1.00	7.56	6	6
ATOM	1924	CA	HIS A 235	41.640	23.999	40.796	1.00	6.75	6	6	ATOM	1978	N	LEU A 241	31.251	25.631	47.191	1.00	7.63	8	8
ATOM	1925	CB	HIS A 235	42.497	25.195	40.296	1.00	6.58	6	6	ATOM	1979	CA	LEU A 241	32.639	24.464	45.838	1.00	7.46	7	7
ATOM	1926	CG	HIS A 235	43.030	24.789	38.959	1.00	6.14	6	6	ATOM	1980	CG	LEU A 241	31.880	24.877	44.661	1.00	7.91	6	6
ATOM	1927	CD2	HIS A 235	42.575	25.085	37.724	1.00	7.29	6	6	ATOM	1981	CG	LEU A 241	32.528	24.553	43.318	1.00	5.00	6	6
ATOM	1928	HD1	HIS A 235	44.084	23.935	38.789	1.00	5.80	7	7	ATOM	1982	CD1	LEU A 241	33.814	25.279	42.944	1.00	5.00	6	6
ATOM	1929	CE1	HIS A 235	44.290	23.756	37.502	1.00	7.11	6	6	ATOM	1983	CD2	LEU A 241	34.520	24.613	41.753	1.00	5.00	6	6
ATOM	1930	ME2	HIS A 235	43.386	24.446	36.829	1.00	6.22	7	7	ATOM	1984	C	LEU A 241	33.548	26.754	42.654	1.00	5.00	6	6
ATOM	1931	C	HIS A 235	40.857	24.459	42.002	1.00	6.76	6	6	ATOM	1985	O	LEU A 241	30.418	24.377	44.720	1.00	8.46	6	6
ATOM	1932	O	HIS A 235	41.512	25.042	42.814	1.00	6.54	8	8	ATOM	1986	N	LEU A 241	29.483	25.127	44.303	1.00	8.58	8	8
ATOM	1933	N	ILE A 236	39.583	24.361	42.255	1.00	6.68	7	7	ATOM	1987	CA	ARG A 242	30.184	23.164	45.219	1.00	8.61	7	7
ATOM	1934	CA	ILE A 236	38.916	24.866	43.434	1.00	6.87	6	6	ATOM	1988	CB	ARG A 242	28.777	22.774	45.286	1.00	8.92	6	6
ATOM	1935	CB2	ILE A 236	37.858	25.949	43.026	1.00	5.00	6	6	ATOM	1989	CG	ARG A 242	28.716	21.266	45.431	1.00	10.58	6	6
ATOM	1936	CG1	ILE A 236	37.089	26.450	44.213	1.00	5.00	6	6	ATOM	1990	CG	ARG A 242	28.819	20.546	46.608	1.00	12.57	6	6
ATOM	1937	CG1	ILE A 236	38.558	27.103	42.238	1.00	5.00	6	6	ATOM	1991	ME	ARG A 242	27.687	19.642	47.094	1.00	13.52	6	6
ATOM	1938	CD1	ILE A 236	37.601	27.999	41.485	1.00	5.00	6	6	ATOM	1992	CZ	ARG A 242	28.192	19.629	48.476	1.00	15.26	7	7
ATOM	1939	O	ILE A 236	38.228	23.724	44.193	1.00	7.20	6	6	ATOM	1993	NH1	ARG A 242	28.955	18.913	49.256	1.00	17.48	6	6
ATOM	1940	N	LYS A 237	37.587	22.852	43.555	1.00	7.08	8	8	ATOM	1994	NH2	ARG A 242	29.464	17.761	48.866	1.00	19.52	7	7
ATOM	1941	H	LYS A 237	38.407	23.693	45.498	1.00	7.74	6	6	ATOM	1995	C	ARG A 242	29.303	19.285	50.505	1.00	18.04	7	7
ATOM	1942	CA	LYS A 237	37.831	22.688	46.424	1.00	7.74	6	6	ATOM	1996	O	ARG A 242	28.042	23.548	46.379	1.00	8.91	6	6
ATOM	1943	CB	LYS A 237	37.828	23.257	47.868	1.00	9.45	6	6	ATOM	1997	N	ASP A 243	26.891	23.909	46.129	1.00	8.59	8	8
ATOM	1944	CG	LYS A 237	37.355	22.233	48.831	1.00	12.16	6	6	ATOM	1998	CA	ASP A 243	28.653	23.828	47.526	1.00	9.00	7	7
ATOM	1945	CD	LYS A 237	37.037	22.463	50.263	1.00	15.99	6	6	ATOM	1999	CB	ASP A 243	27.964	24.591	48.533	1.00	9.47	6	6
ATOM	1946	CE	LYS A 237	37.992	23.114	51.189	1.00	19.56	6	6	ATOM	2000	CG	ASP A 243	28.812	24.581	49.811	1.00	11.98	6	6
ATOM	1947	HZ	LYS A 237	37.579	22.767	52.623	1.00	22.41	7	7	ATOM	2001	CD1	ASP A 243	28.766	23.183	50.417	1.00	15.20	6	6
ATOM	1948	C	LYS A 237	36.425	22.314	45.956	1.00	7.39	6	6	ATOM	2002	CD2	ASP A 243	29.580	22.982	51.372	1.00	19.21	8	8
ATOM	1949	O	LYS A 237	35.561	23.187	45.849	1.00	6.92	8	8	ATOM	2003	C	ASP A 243	28.049	22.251	50.036	1.00	13.33	8	8
ATOM	1950	N	PHE A 238	36.210	21.062	45.551	1.00	7.45	7	7	ATOM	2004	O	ASP A 243	27.798	26.049	48.117	1.00	9.53	6	6
ATOM	1951	CA	PHE A 238	34.912	20.689	44.944	1.00	7.67	6	6	ATOM	2005	N	TRP A 244	26.797	26.664	48.539	1.00	9.34	8	8
ATOM	1952	CB	PHE A 238	34.921	19.232	44.425	1.00	8.77	6	6	ATOM	2006	CA	TRP A 244	28.755	26.581	47.303	1.00	9.34	8	8
ATOM	1953	CG	PHE A 238	35.992	18.884	43.442	1.00	9.75	6	6	ATOM	2007	CB	TRP A 244	28.622	28.005	46.908	1.00	9.20	6	6
ATOM	1954	CD1	PHE A 238	36.688	19.851	42.716	1.00	10.39	6	6	ATOM	2008	CG	TRP A 244	29.862	28.511	46.195	1.00	7.34	6	6
ATOM	1955	CD2	PHE A 238	36.262	17.529	43.199	1.00	10.39	6	6	ATOM	2009	CD2	TRP A 244	29.831	29.924	45.719	1.00	8.91	6	6
ATOM	1956	CE1	PHE A 238	37.638	17.448	41.787	1.00	9.12	6	6	ATOM	2010	CE2	TRP A 244	29.442	30.367	44.411	1.00	9.51	6	6
ATOM	1957	CE2	PHE A 238	37.220	17.125	42.292	1.00	8.83	6	6	ATOM	2011	CE3	TRP A 244	29.589	31.773	44.384	1.00	10.54	6	6
ATOM	1958	C2	PHE A 238	37.882	18.097	41.562	1.00	9.31	6	6	ATOM	2012	CE4	TRP A 244	29.020	29.698	43.243	1.00	10.38	6	6
ATOM	1959	C	PHE A 238	33.694	20.870	45.841	1.00	7.61	8	8	ATOM	2013	NE1	TRP A 244	30.168	31.065	46.419	1.00	9.07	6	6
ATOM	1960	O	PHE A 238	32.666	21.356	45.350	1.00	7.47	8	8	ATOM	2014	C22	TRP A 244	30.036	32.191	45.638	1.00	9.59	7	7
ATOM	1961	N	SER A 239	33.801	20.475	47.113	1.00	7.50	7	7					29.289	32.524	43.219	1.00	9.81	6	6

ATOM	2015	C23	TRP	A	244	28.727	30.446	42.096	1.00	10.45	6
ATOM	2016	CH2	TRP	A	244	28.862	31.859	42.106	1.00	9.71	6
ATOM	2017	C	TRP	A	244	27.386	28.200	46.006	1.00	9.28	6
ATOM	2018	O	TRP	A	244	26.651	29.168	46.164	1.00	8.82	8
ATOM	2019	N	VAL	A	245	27.217	27.284	45.056	1.00	9.64	7
ATOM	2020	CA	VAL	A	245	26.082	27.305	44.114	1.00	10.52	6
ATOM	2021	CB	VAL	A	245	26.108	26.185	43.039	1.00	12.05	6
ATOM	2022	CG1	VAL	A	245	24.832	26.113	42.198	1.00	13.84	6
ATOM	2023	CG2	VAL	A	245	27.262	26.450	42.081	1.00	13.35	6
ATOM	2024	C	VAL	A	245	24.722	27.203	44.853	1.00	10.62	6
ATOM	2025	O	VAL	A	245	23.758	27.906	44.590	1.00	10.03	7
ATOM	2026	N	GLN	A	246	24.745	26.269	45.790	1.00	11.30	7
ATOM	2027	CA	GLN	A	246	23.552	26.022	46.634	1.00	12.37	6
ATOM	2028	CB	GLN	A	246	23.878	24.727	47.381	1.00	18.96	6
ATOM	2029	CG	GLN	A	246	22.737	24.176	48.214	1.00	27.47	6
ATOM	2030	CD	GLN	A	246	22.842	23.446	50.493	1.00	36.63	6
ATOM	2031	OE1	GLN	A	246	24.476	22.642	49.028	1.00	36.61	7
ATOM	2032	ME2	GLN	A	246	23.153	27.225	47.485	1.00	12.22	8
ATOM	2033	C	GLN	A	246	21.970	27.561	47.531	1.00	12.47	6
ATOM	2034	O	GLN	A	246	24.083	27.968	48.099	1.00	12.46	6
ATOM	2035	N	ALA	A	247	23.852	29.144	48.893	1.00	12.61	6
ATOM	2036	CA	ALA	A	247	25.094	29.791	49.517	1.00	12.47	6
ATOM	2037	CB	ALA	A	247	23.231	30.263	48.050	1.00	12.74	6
ATOM	2038	C	ALA	A	247	22.308	30.857	48.561	1.00	12.85	8
ATOM	2039	O	ALA	A	247	23.710	30.495	46.838	1.00	12.75	7
ATOM	2040	N	VAL	A	248	23.159	31.471	45.913	1.00	12.69	6
ATOM	2041	CA	VAL	A	248	24.009	31.688	44.684	1.00	11.87	6
ATOM	2042	CB	VAL	A	248	23.357	32.721	43.754	1.00	11.19	6
ATOM	2043	CG1	VAL	A	248	25.400	32.171	45.014	1.00	11.42	6
ATOM	2044	CG2	VAL	A	248	21.748	31.040	45.337	1.00	12.91	6
ATOM	2045	C	VAL	A	248	20.866	31.889	45.506	1.00	12.81	8
ATOM	2046	N	ARG	A	249	21.483	29.791	45.237	1.00	13.31	7
ATOM	2047	O	ARG	A	249	20.124	29.352	44.897	1.00	13.92	6
ATOM	2048	CA	ARG	A	249	20.066	27.906	44.404	1.00	11.75	6
ATOM	2049	CB	ARG	A	249	20.814	27.726	43.033	1.00	12.59	6
ATOM	2050	CG	ARG	A	249	21.411	26.198	41.224	1.00	13.02	7
ATOM	2051	CD	ARG	A	249	22.045	25.161	40.739	1.00	13.82	6
ATOM	2052	HE	ARG	A	249	22.150	24.041	41.476	1.00	11.68	7
ATOM	2053	C2	ARG	A	249	22.589	25.166	39.515	1.00	15.22	7
ATOM	2054	HU1	ARG	A	249	19.215	29.503	46.125	1.00	14.55	6
ATOM	2055	HU2	ARG	A	249	18.082	30.005	45.970	1.00	14.34	8
ATOM	2056	O	ARG	A	249	19.685	29.106	47.329	1.00	15.16	7
ATOM	2057	C	ARG	A	249	18.794	29.252	48.498	1.00	15.83	6
ATOM	2058	N	GLM	A	250	19.437	28.816	49.790	1.00	21.15	6
ATOM	2059	CA	GLM	A	250	18.902	27.566	50.460	1.00	28.24	6
ATOM	2060	CG	GLM	A	250	20.067	26.619	50.807	1.00	32.12	6
ATOM	2061	CD	GLM	A	250	21.116	27.047	51.333	1.00	34.30	8
ATOM	2062	CE1	GLM	A	250	19.907	25.331	50.478	1.00	32.80	7
ATOM	2063	CE2	GLM	A	250	18.362	30.699	48.707	1.00	15.86	6
ATOM	2064	HE2	GLM	A	250	17.196	31.022	48.871	1.00	15.83	8
ATOM	2065	C	GLM	A	250	19.316	31.621	48.689	1.00	15.85	7
ATOM	2066	O	GLM	A	250						
ATOM	2067	N	ALA	A	251						
ATOM	2068	CA	ALA	A	251	19.029	33.029	48.862	1.00	16.06	6
ATOM	2069	CB	ALA	A	251	20.374	33.774	48.984	1.00	16.48	6
ATOM	2070	C	ALA	A	251	18.276	33.749	47.765	1.00	16.26	6
ATOM	2071	O	ALA	A	251	17.596	34.738	48.088	1.00	16.47	8
ATOM	2072	N	THR	A	252	18.343	33.433	46.476	1.00	16.21	7
ATOM	2073	CA	THR	A	252	17.631	34.224	45.487	1.00	16.03	6
ATOM	2074	CB	THR	A	252	18.462	34.328	44.189	1.00	13.96	6
ATOM	2075	CG1	THR	A	252	18.697	32.968	43.824	1.00	11.77	8
ATOM	2076	CG2	THR	A	252	19.776	35.060	44.281	1.00	12.34	6
ATOM	2077	C	THR	A	252	16.292	33.577	45.170	1.00	16.40	6
ATOM	2078	O	THR	A	252	15.441	34.281	44.670	1.00	16.40	8
ATOM	2079	N	GLY	A	253	16.139	32.267	45.429	1.00	16.68	7
ATOM	2080	CA	GLY	A	253	14.955	31.502	45.168	1.00	16.75	6
ATOM	2081	C	GLY	A	253	14.963	31.170	43.660	1.00	17.06	6
ATOM	2082	O	GLY	A	253	13.985	30.602	43.167	1.00	17.16	8
ATOM	2083	N	LYS	A	254	16.018	31.475	42.888	1.00	17.07	7
ATOM	2084	CA	LYS	A	254	16.045	31.196	41.437	1.00	16.76	6
ATOM	2085	CB	LYS	A	254	16.734	32.377	40.748	1.00	18.37	6
ATOM	2086	CG	LYS	A	254	16.007	33.685	40.568	1.00	21.23	6
ATOM	2087	CD	LYS	A	254	16.884	34.884	40.536	1.00	23.96	6
ATOM	2088	CE	LYS	A	254	17.330	35.674	39.332	1.00	25.51	6
ATOM	2089	NZ	LYS	A	254	18.369	36.723	39.792	1.00	27.00	7
ATOM	2090	C	LYS	A	254	16.731	29.871	41.097	1.00	16.34	6
ATOM	2091	O	LYS	A	254	17.533	29.323	41.896	1.00	16.45	8
ATOM	2092	N	GLU	A	255	16.459	29.313	39.928	1.00	15.71	7
ATOM	2093	CA	GLU	A	255	17.084	28.072	39.466	1.00	15.30	6
ATOM	2094	CB	GLU	A	255	16.504	27.668	38.102	1.00	18.71	6
ATOM	2095	CG	GLU	A	255	16.954	26.337	37.542	1.00	24.80	6
ATOM	2096	CD	GLU	A	255	16.927	26.270	36.020	1.00	29.50	6
ATOM	2097	OE1	GLU	A	255	16.083	26.965	35.393	1.00	31.45	8
ATOM	2098	OE2	GLU	A	255	17.730	25.553	35.340	1.00	31.98	8
ATOM	2099	C	GLU	A	255	18.623	28.183	39.365	1.00	14.27	6
ATOM	2100	O	GLU	A	255	19.417	27.324	39.733	1.00	14.14	8
ATOM	2101	N	MET	A	256	19.098	29.303	38.859	1.00	13.25	7
ATOM	2102	CA	MET	A	256	20.476	29.628	38.676	1.00	12.49	6
ATOM	2103	CB	MET	A	256	21.171	29.970	39.998	1.00	12.38	6
ATOM	2104	CG	MET	A	256	20.740	31.237	40.705	1.00	13.41	6
ATOM	2105	SD	MET	A	256	20.539	32.774	39.751	1.00	13.00	16
ATOM	2106	CE	MET	A	256	22.245	33.221	39.432	1.00	12.60	6
ATOM	2107	C	MET	A	256	21.209	28.486	37.966	1.00	11.87	6
ATOM	2108	O	MET	A	256	22.065	27.824	38.595	1.00	11.99	8
ATOM	2109	N	PHE	A	257	20.904	28.261	36.696	1.00	10.99	7
ATOM	2110	CA	PHE	A	257	21.612	27.238	35.914	1.00	10.24	6
ATOM	2111	CB	PHE	A	257	21.254	27.347	36.397	1.00	9.31	6
ATOM	2112	CG	PHE	A	257	22.056	26.339	33.591	1.00	9.08	6
ATOM	2113	CD1	PHE	A	257	21.634	25.032	33.491	1.00	8.44	6
ATOM	2114	CD2	PHE	A	257	23.248	26.741	32.991	1.00	7.86	6
ATOM	2115	CE1	PHE	A	257	22.425	26.132	32.769	1.00	9.31	6
ATOM	2116	CE2	PHE	A	257	24.059	25.861	32.292	1.00	9.08	6
ATOM	2117	CZ	PHE	A	257	23.624	24.537	32.171	1.00	10.03	6
ATOM	2118	C	PHE	A	257	23.115	27.439	36.047	1.00	9.70	6
ATOM	2119	O	PHE	A	257	23.583	28.593	35.876	1.00	9.75	8
ATOM	2120	N	THR	A	258	23.933	26.447	36.329	1.00	9.20	7

SUBSTITUTE SHEET (RULE 26)

ATOM	2121	CA	THR A 258	25.392	26.609	36.450	1.00	8.71	6	ATOM	2174	N	GLM A 264	39.758	18.950	31.301	1.00	10.57	7
ATOM	2122	CB	THR A 258	25.824	26.583	37.938	1.00	8.83	6	ATOM	2175	CA	GLM A 264	40.441	17.687	31.185	1.00	10.92	6
ATOM	2123	OG1	THR A 258	25.203	27.078	38.617	1.00	7.38	8	ATOM	2176	CB	GLM A 264	40.619	16.999	32.536	1.00	14.66	6
ATOM	2124	CG2	THR A 258	27.337	26.720	38.142	1.00	8.42	6	ATOM	2177	CG	GLM A 264	41.796	16.043	32.600	1.00	18.65	6
ATOM	2125	C	THR A 258	26.136	25.533	35.666	1.00	8.29	6	ATOM	2178	CD	GLM A 264	41.972	15.344	33.934	1.00	22.60	6
ATOM	2126	O	THR A 258	25.764	24.361	35.606	1.00	8.22	8	ATOM	2179	OE1	GLM A 264	41.214	15.481	36.907	1.00	26.23	8
ATOM	2127	N	VAL A 259	27.160	25.972	34.922	1.00	7.82	7	ATOM	2180	HE2	GLM A 264	42.996	14.478	34.047	1.00	23.90	7
ATOM	2128	CA	VAL A 259	28.001	25.077	34.102	1.00	7.47	6	ATOM	2181	C	GLM A 264	39.681	16.811	30.191	1.00	11.04	6
ATOM	2129	CB	VAL A 259	27.859	25.175	32.564	1.00	5.00	6	ATOM	2182	O	GLM A 264	38.461	16.643	30.232	1.00	10.83	8
ATOM	2130	OG1	VAL A 259	28.101	26.589	32.036	1.00	5.00	6	ATOM	2183	N	ASN A 265	40.454	16.216	29.289	1.00	11.25	7
ATOM	2131	CG2	VAL A 259	28.799	24.202	31.809	1.00	5.00	6	ATOM	2184	CA	ASN A 265	40.151	15.322	28.209	1.00	11.87	6
ATOM	2132	C	VAL A 259	29.428	25.381	34.552	1.00	7.58	6	ATOM	2185	CB	ASN A 265	41.223	15.365	27.078	1.00	11.52	6
ATOM	2133	O	VAL A 259	29.821	26.552	36.634	1.00	7.78	8	ATOM	2186	CG	ASN A 265	40.655	14.637	25.854	1.00	12.03	6
ATOM	2134	N	ALA A 260	30.181	24.348	36.913	1.00	7.84	7	ATOM	2187	CO1	ASN A 265	39.485	14.278	25.764	1.00	11.79	8
ATOM	2135	CA	ALA A 260	31.555	24.487	35.366	1.00	8.08	6	ATOM	2188	WD2	ASN A 265	41.445	14.294	28.857	1.00	11.74	7
ATOM	2136	CB	ALA A 260	31.982	23.621	36.534	1.00	7.64	6	ATOM	2189	C	ASN A 265	40.028	13.873	28.691	1.00	12.36	6
ATOM	2137	C	ALA A 260	32.523	24.076	36.215	1.00	8.28	6	ATOM	2190	O	ASN A 265	40.755	13.007	28.282	1.00	12.25	8
ATOM	2138	O	ALA A 260	32.266	23.091	33.536	1.00	8.26	8	ATOM	2191	N	ASN A 266	39.116	13.676	29.634	1.00	13.06	7
ATOM	2139	N	GLU A 261	33.579	24.848	34.057	1.00	8.40	7	ATOM	2192	CA	ASN A 266	38.844	12.428	30.337	1.00	13.75	6
ATOM	2140	CA	GLU A 261	34.628	24.574	33.125	1.00	8.60	6	ATOM	2193	CB	ASN A 266	39.910	12.362	31.416	1.00	18.58	6
ATOM	2141	CB	GLU A 261	35.346	25.828	32.600	1.00	11.43	6	ATOM	2194	CG	ASN A 266	40.150	11.016	32.031	1.00	22.56	6
ATOM	2142	CG	GLU A 261	36.281	25.350	31.518	1.00	17.13	6	ATOM	2195	CO1	ASN A 266	41.311	10.519	31.969	1.00	26.43	8
ATOM	2143	OE1	GLU A 261	36.823	26.339	30.525	1.00	23.18	6	ATOM	2196	WD2	ASN A 266	39.160	10.410	32.662	1.00	21.13	7
ATOM	2144	DE2	GLU A 261	36.068	26.970	29.694	1.00	25.81	8	ATOM	2197	C	ASN A 266	37.441	12.394	30.944	1.00	13.73	6
ATOM	2145	OE1	GLU A 261	38.080	26.441	30.593	1.00	25.35	8	ATOM	2198	O	ASN A 266	37.161	13.123	31.927	1.00	13.68	8
ATOM	2146	C	GLU A 261	35.644	23.659	33.867	1.00	8.48	6	ATOM	2199	N	ALA A 267	36.552	11.545	30.362	1.00	13.47	7
ATOM	2147	O	GLU A 261	36.514	24.148	34.558	1.00	8.19	8	ATOM	2200	CA	ALA A 267	35.178	11.440	30.835	1.00	13.35	6
ATOM	2148	N	TYR A 262	35.578	22.360	33.730	1.00	8.54	7	ATOM	2201	CB	ALA A 267	34.330	10.522	29.944	1.00	12.56	6
ATOM	2149	CA	TYR A 262	36.500	21.387	33.293	1.00	8.87	6	ATOM	2202	C	ALA A 267	35.076	10.997	32.287	1.00	13.08	6
ATOM	2150	CB	TYR A 262	35.838	20.183	34.966	1.00	8.94	6	ATOM	2203	O	ALA A 267	34.195	11.454	33.027	1.00	13.14	8
ATOM	2151	CG	TYR A 262	36.761	19.321	35.821	1.00	9.11	6	ATOM	2204	N	GLY A 268	35.918	10.106	32.733	1.00	12.97	7
ATOM	2152	CD1	TYR A 262	36.660	19.322	37.206	1.00	9.01	6	ATOM	2205	CA	GLY A 268	35.973	9.564	34.083	1.00	12.93	6
ATOM	2153	CD2	TYR A 262	37.509	18.576	37.984	1.00	9.15	6	ATOM	2206	C	GLY A 268	36.184	10.653	35.146	1.00	13.05	6
ATOM	2154	CD2	TYR A 262	37.743	18.497	35.253	1.00	9.44	6	ATOM	2207	O	GLY A 268	35.512	10.656	36.213	1.00	13.01	8
ATOM	2155	CE2	TYR A 262	38.605	17.723	36.026	1.00	9.65	6	ATOM	2208	N	LYS A 269	37.109	11.575	34.879	1.00	12.90	7
ATOM	2156	C2	TYR A 262	38.690	17.788	37.415	1.00	9.42	6	ATOM	2209	CA	LYS A 269	37.425	12.681	35.786	1.00	13.04	6
ATOM	2157	OH	TYR A 262	39.305	17.012	38.214	1.00	9.41	8	ATOM	2210	CB	LYS A 269	38.790	13.296	35.417	1.00	17.83	6
ATOM	2158	C	TYR A 262	37.624	20.977	33.104	1.00	8.97	6	ATOM	2211	CB	LYS A 269	39.840	12.506	36.217	1.00	22.85	6
ATOM	2159	O	TYR A 262	37.008	20.107	32.297	1.00	9.09	8	ATOM	2212	CD	LYS A 269	40.869	12.034	35.211	1.00	27.74	6
ATOM	2160	N	TRP A 263	38.590	21.592	32.945	1.00	9.15	7	ATOM	2213	CE	LYS A 269	41.722	10.885	35.785	1.00	30.85	6
ATOM	2161	CA	TRP A 263	39.603	21.292	31.774	1.00	9.76	6	ATOM	2214	W2	LYS A 269	42.663	10.356	34.698	1.00	32.23	7
ATOM	2162	CB	TRP A 263	40.183	22.560	31.346	1.00	9.45	6	ATOM	2215	C	LYS A 269	36.296	13.699	35.776	1.00	12.76	6
ATOM	2163	CG	TRP A 263	40.638	22.366	29.917	1.00	11.66	6	ATOM	2216	O	LYS A 269	35.918	14.230	36.828	1.00	12.65	8
ATOM	2164	CD2	TRP A 263	39.892	22.703	28.733	1.00	12.75	6	ATOM	2217	N	LEU A 270	35.696	13.903	34.596	1.00	12.42	7
ATOM	2165	CE2	TRP A 263	40.662	22.899	27.612	1.00	13.78	6	ATOM	2218	CA	LEU A 270	34.539	16.810	34.538	1.00	12.16	6
ATOM	2166	CE3	TRP A 263	38.631	23.289	28.512	1.00	10.24	6	ATOM	2219	CB	LEU A 270	34.164	15.161	33.088	1.00	13.49	6
ATOM	2167	CD1	TRP A 263	41.800	21.810	29.466	1.00	12.57	7	ATOM	2220	CD	LEU A 270	34.614	17.623	33.197	1.00	13.42	6
ATOM	2168	NE1	TRP A 263	41.820	21.731	28.078	1.00	13.80	6	ATOM	2221	CO1	LEU A 270	36.465	16.210	32.550	1.00	13.72	6
ATOM	2169	C22	TRP A 263	40.205	22.513	26.299	1.00	14.12	6	ATOM	2222	C2	LEU A 270	33.412	14.169	35.315	1.00	11.76	6
ATOM	2170	C23	TRP A 263	38.201	23.453	27.210	1.00	10.77	6	ATOM	2223	O	LEU A 270	32.700	14.934	35.981	1.00	11.63	8
ATOM	2171	CH2	TRP A 263	38.970	23.094	26.122	1.00	11.88	6	ATOM	2224	O	LEU A 270	33.219	12.851	35.281	1.00	11.41	7
ATOM	2172	C	TRP A 263	40.303	20.053	31.833	1.00	10.24	6	ATOM	2225	N	GLU A 271	32.136	12.233	36.051	1.00	11.29	6
ATOM	2173	O	TRP A 263	41.436	20.018	32.294	1.00	10.30	8										

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ATOM	2227	CB	GLU A 271	32.024	10.817	35.510	1.00	16.08	6
ATOM	2228	CG	GLU A 271	31.015	10.010	36.333	1.00	23.09	6
ATOM	2229	CG	GLU A 271	30.861	8.627	35.720	1.00	27.19	6
ATOM	2230	OE1	GLU A 271	29.716	8.351	35.359	1.00	29.23	8
ATOM	2231	OE2	GLU A 271	31.830	7.845	35.526	1.00	30.01	8
ATOM	2232	C	GLU A 271	32.339	12.279	37.554	1.00	10.89	6
ATOM	2233	O	GLU A 271	31.458	12.370	38.404	1.00	10.58	8
ATOM	2234	N	ASN A 272	33.615	12.189	37.987	1.00	10.66	7
ATOM	2235	CA	ASN A 272	34.008	12.309	39.105	1.00	10.31	6
ATOM	2236	CB	ASN A 272	35.520	12.089	39.643	1.00	11.32	6
ATOM	2237	CG	ASN A 272	35.969	12.380	41.064	1.00	11.99	6
ATOM	2238	CD1	ASN A 272	35.616	11.603	41.966	1.00	11.66	8
ATOM	2239	ND2	ASN A 272	36.701	13.474	41.322	1.00	12.45	7
ATOM	2240	C	ASN A 272	33.588	13.709	39.873	1.00	9.78	6
ATOM	2241	O	ASN A 272	33.080	13.897	40.979	1.00	9.63	8
ATOM	2242	N	TYR A 273	33.777	14.748	39.063	1.00	9.45	7
ATOM	2243	CA	TYR A 273	33.349	16.104	39.486	1.00	9.06	6
ATOM	2244	CB	TYR A 273	33.908	17.179	38.558	1.00	8.65	6
ATOM	2245	CG	TYR A 273	33.509	18.626	38.903	1.00	8.44	6
ATOM	2246	CD1	TYR A 273	34.242	19.333	39.838	1.00	8.51	6
ATOM	2247	CE1	TYR A 273	33.915	20.650	40.228	1.00	8.39	6
ATOM	2248	CD2	TYR A 273	32.391	19.231	38.364	1.00	8.33	6
ATOM	2249	CE2	TYR A 273	32.015	20.523	38.695	1.00	8.66	6
ATOM	2250	C2	TYR A 273	32.827	21.214	39.625	1.00	8.60	6
ATOM	2251	OH	TYR A 273	32.452	22.481	39.938	1.00	8.94	8
ATOM	2252	C	TYR A 273	31.837	16.135	39.662	1.00	9.06	6
ATOM	2253	O	TYR A 273	31.340	16.679	40.688	1.00	8.80	8
ATOM	2254	N	LEU A 274	31.061	15.569	38.736	1.00	9.52	7
ATOM	2255	CA	LEU A 274	29.590	15.550	38.849	1.00	10.16	6
ATOM	2256	CB	LEU A 274	28.901	14.856	37.646	1.00	10.22	6
ATOM	2257	CG	LEU A 274	29.158	15.528	36.280	1.00	10.91	6
ATOM	2258	CD1	LEU A 274	28.719	14.634	35.107	1.00	11.67	6
ATOM	2259	CD2	LEU A 274	28.432	16.843	36.198	1.00	10.03	6
ATOM	2260	C	LEU A 274	29.157	14.918	40.173	1.00	10.59	6
ATOM	2261	O	LEU A 274	28.353	15.463	40.920	1.00	10.27	8
ATOM	2262	N	ASN A 275	29.706	13.730	40.471	1.00	11.45	7
ATOM	2263	CA	ASN A 275	29.463	13.009	41.709	1.00	12.37	6
ATOM	2264	CB	ASN A 275	30.287	11.694	41.835	1.00	19.11	6
ATOM	2265	CG	ASN A 275	29.761	10.565	40.962	1.00	24.07	6
ATOM	2266	CD1	ASN A 275	28.743	9.915	41.314	1.00	27.53	8
ATOM	2267	ND2	ASN A 275	30.352	10.254	39.805	1.00	23.40	7
ATOM	2268	C	ASN A 275	29.820	13.870	42.924	1.00	12.36	6
ATOM	2269	O	ASN A 275	28.964	14.072	43.761	1.00	12.19	8
ATOM	2270	N	LYS A 276	31.008	14.435	43.005	1.00	12.51	7
ATOM	2271	CA	LYS A 276	31.461	15.251	44.130	1.00	12.99	6
ATOM	2272	CB	LYS A 276	32.952	15.605	44.000	1.00	12.82	6
ATOM	2273	CG	LYS A 276	33.825	14.346	44.050	1.00	13.95	6
ATOM	2274	CD	LYS A 276	33.535	13.485	45.269	1.00	14.29	6
ATOM	2275	CE	LYS A 276	34.141	12.103	45.203	1.00	13.18	6
ATOM	2276	H2	LYS A 276	35.602	12.070	44.906	1.00	13.50	7
ATOM	2277	C	LYS A 276	30.651	16.533	44.311	1.00	13.75	8
ATOM	2278	O	LYS A 276	30.650	17.117	45.412	1.00	13.75	8
ATOM	2279	N	THR A 277	29.966	16.979	43.256	1.00	12.99	7
ATOM	2280	CA	THR A 277	29.173	18.187	43.406	1.00	12.78	6
ATOM	2281	CB	THR A 277	29.520	19.264	42.357	1.00	12.02	6
ATOM	2282	OG1	THR A 277	29.323	18.649	41.065	1.00	12.30	8
ATOM	2283	CG2	THR A 277	30.941	19.791	42.492	1.00	8.90	6
ATOM	2284	C	THR A 277	27.701	17.794	43.416	1.00	12.70	6
ATOM	2285	O	THR A 277	26.812	18.613	43.190	1.00	12.66	8
ATOM	2286	N	SER A 278	27.426	16.518	43.673	1.00	12.73	7
ATOM	2287	CA	SER A 278	26.069	16.047	43.729	1.00	12.63	6
ATOM	2288	CB	SER A 278	25.280	16.806	44.854	1.00	14.69	6
ATOM	2289	OG	SER A 278	25.963	16.531	46.061	1.00	18.04	8
ATOM	2290	C	SER A 278	25.283	16.294	42.474	1.00	12.85	6
ATOM	2291	O	SER A 278	24.049	16.483	42.663	1.00	13.07	8
ATOM	2292	N	PIE A 279	25.774	16.339	41.260	1.00	12.49	7
ATOM	2293	CA	PIE A 279	24.897	16.593	40.100	1.00	12.16	6
ATOM	2294	CB	PIE A 279	23.976	15.346	39.973	1.00	12.70	6
ATOM	2295	CG	PIE A 279	24.772	14.122	39.524	1.00	12.87	6
ATOM	2296	CD1	PIE A 279	25.183	13.153	40.435	1.00	13.85	6
ATOM	2297	CD2	PIE A 279	25.085	13.919	38.199	1.00	13.30	6
ATOM	2298	CE1	PIE A 279	25.903	12.038	40.045	1.00	13.14	6
ATOM	2299	CE2	PIE A 279	25.801	12.799	37.786	1.00	13.99	6
ATOM	2300	C2	PIE A 279	26.266	11.878	38.726	1.00	13.30	6
ATOM	2301	C	PIE A 279	24.170	17.912	40.149	1.00	12.03	6
ATOM	2302	O	PIE A 279	23.185	18.072	39.417	1.00	12.27	8
ATOM	2303	N	ASN A 280	24.646	18.942	40.882	1.00	11.58	7
ATOM	2304	CA	ASN A 280	23.979	20.228	40.984	1.00	11.30	6
ATOM	2305	CB	ASN A 280	24.025	20.735	42.438	1.00	11.18	6
ATOM	2306	CG	ASN A 280	25.222	21.558	42.868	1.00	13.48	6
ATOM	2307	CD1	ASN A 280	26.142	21.809	42.087	1.00	12.89	8
ATOM	2308	ND2	ASN A 280	25.289	22.094	44.111	1.00	12.18	7
ATOM	2309	C	ASN A 280	24.422	21.247	39.927	1.00	10.94	6
ATOM	2310	O	ASN A 280	23.910	22.353	39.820	1.00	11.03	8
ATOM	2311	N	GLN A 281	25.325	20.890	39.032	1.00	10.60	7
ATOM	2312	CA	GLN A 281	25.784	21.736	37.949	1.00	10.04	6
ATOM	2313	CB	GLN A 281	26.930	22.636	38.400	1.00	9.98	6
ATOM	2314	CG	GLN A 281	28.117	21.977	39.038	1.00	9.72	6
ATOM	2315	CD	GLN A 281	29.055	22.863	39.859	1.00	9.00	6
ATOM	2316	OE1	GLN A 281	30.064	23.342	39.350	1.00	8.97	8
ATOM	2317	NE2	GLN A 281	28.835	23.085	41.151	1.00	8.05	7
ATOM	2318	C	GLN A 281	26.239	20.871	36.771	1.00	9.46	6
ATOM	2319	O	GLN A 281	26.615	19.703	36.902	1.00	9.22	8
ATOM	2320	N	SER A 282	26.224	21.522	35.616	1.00	9.14	7
ATOM	2321	CA	SER A 282	26.674	20.851	34.389	1.00	8.74	6
ATOM	2322	CB	SER A 282	25.985	21.419	33.131	1.00	7.22	6
ATOM	2323	OG	SER A 282	24.607	21.123	33.102	1.00	6.53	8
ATOM	2324	C	SER A 282	28.170	21.077	34.201	1.00	8.54	6
ATOM	2325	O	SER A 282	28.773	21.913	34.919	1.00	8.89	8
ATOM	2326	N	VAL A 283	28.777	20.420	33.240	1.00	8.11	7
ATOM	2327	CA	VAL A 283	30.154	20.596	32.841	1.00	7.98	6
ATOM	2328	CB	VAL A 283	31.137	19.443	33.210	1.00	8.54	6
ATOM	2329	CG1	VAL A 283	31.457	19.441	34.708	1.00	9.20	6
ATOM	2330	CG2	VAL A 283	30.599	18.117	32.719	1.00	7.85	6
ATOM	2331	C	VAL A 283	30.218	20.758	31.304	1.00	7.87	6
ATOM	2332	O	VAL A 283	29.342	20.265	30.572	1.00	7.75	8

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ATOM	2333	N	PHE A 284	31.212	21.483	30.801	1.00	7.72	7
ATOM	2334	CA	PHE A 284	31.460	21.589	29.383	1.00	7.67	6
ATOM	2335	CB	PHE A 284	32.518	22.649	29.110	1.00	7.48	6
ATOM	2336	CD	PHE A 284	31.953	24.040	29.240	1.00	7.61	6
ATOM	2337	CE	PHE A 284	32.301	24.886	30.277	1.00	6.90	6
ATOM	2338	CE1	PHE A 284	31.062	24.475	28.252	1.00	7.80	6
ATOM	2339	CE2	PHE A 284	31.782	26.167	30.312	1.00	8.33	6
ATOM	2340	CE3	PHE A 284	30.501	25.756	28.282	1.00	6.48	6
ATOM	2341	CZ	PHE A 284	30.882	26.602	29.314	1.00	7.74	6
ATOM	2342	C	PHE A 284	31.997	20.212	28.924	1.00	7.86	6
ATOM	2343	O	PHE A 284	32.833	19.541	29.627	1.00	7.52	8
ATOM	2344	N	ASP A 285	31.517	19.758	27.741	1.00	7.99	7
ATOM	2345	CA	ASP A 285	31.997	18.452	27.212	1.00	8.11	6
ATOM	2346	CB	ASP A 285	30.919	17.867	26.269	1.00	8.64	6
ATOM	2347	CG	ASP A 285	31.063	16.361	26.096	1.00	9.93	6
ATOM	2348	CD	ASP A 285	32.173	15.774	26.289	1.00	8.07	8
ATOM	2349	CE	ASP A 285	30.026	15.731	25.769	1.00	9.24	8
ATOM	2350	C	ASP A 285	33.339	18.591	26.496	1.00	8.25	6
ATOM	2351	O	ASP A 285	33.394	18.729	25.236	1.00	8.58	8
ATOM	2352	N	VAL A 286	34.468	18.590	27.218	1.00	7.95	7
ATOM	2353	CA	VAL A 286	35.813	18.709	26.644	1.00	7.75	6
ATOM	2354	CB	VAL A 286	36.851	18.934	27.764	1.00	7.80	6
ATOM	2355	CG	VAL A 286	38.270	19.085	27.261	1.00	5.55	6
ATOM	2356	CD	VAL A 286	36.418	20.221	28.524	1.00	8.40	6
ATOM	2357	C	VAL A 286	36.145	17.549	25.719	1.00	7.74	6
ATOM	2358	O	VAL A 286	36.611	17.833	24.601	1.00	7.94	8
ATOM	2359	N	PRO A 287	35.967	16.276	26.097	1.00	7.41	7
ATOM	2360	CD	PRO A 287	35.495	15.854	25.771	1.00	7.11	6
ATOM	2361	CA	PRO A 287	36.262	15.131	25.226	1.00	7.24	6
ATOM	2362	CB	PRO A 287	35.802	13.885	25.970	1.00	7.14	6
ATOM	2363	CG	PRO A 287	35.741	14.357	27.396	1.00	7.12	6
ATOM	2364	C	PRO A 287	35.589	15.313	23.873	1.00	7.43	6
ATOM	2365	O	PRO A 287	36.214	15.113	22.834	1.00	7.51	8
ATOM	2366	N	LEU A 288	34.293	15.681	23.762	1.00	7.47	7
ATOM	2367	CA	LEU A 288	33.608	15.904	22.504	1.00	7.34	6
ATOM	2368	CB	LEU A 288	32.149	16.325	22.654	1.00	7.25	6
ATOM	2369	CG	LEU A 288	31.430	16.481	21.283	1.00	8.35	6
ATOM	2370	CD	LEU A 288	31.384	15.185	20.494	1.00	8.34	6
ATOM	2371	CE	LEU A 288	30.038	16.988	21.510	1.00	5.28	6
ATOM	2372	C	LEU A 288	34.329	16.998	21.722	1.00	7.39	6
ATOM	2373	O	LEU A 288	34.398	16.793	20.525	1.00	7.49	8
ATOM	2374	N	HIS A 289	34.847	18.097	22.260	1.00	7.34	7
ATOM	2375	CA	HIS A 289	35.583	19.114	21.525	1.00	7.21	6
ATOM	2376	CB	HIS A 289	36.094	20.260	22.445	1.00	5.61	6
ATOM	2377	CG	HIS A 289	37.215	21.083	21.852	1.00	5.00	6
ATOM	2378	CD	HIS A 289	38.548	21.040	22.012	1.00	5.00	6
ATOM	2379	CE	HIS A 289	38.127	22.570	20.527	1.00	5.00	7
ATOM	2380	CE1	HIS A 289	39.124	21.983	21.176	1.00	5.00	7
ATOM	2381	CE2	HIS A 289	36.776	18.507	20.805	1.00	7.52	6
ATOM	2382	C	HIS A 289	37.083	18.809	19.647	1.00	7.41	8
ATOM	2383	O	HIS A 289	37.518	17.654	21.565	1.00	7.75	7
ATOM	2384	N	PHE A 290	38.721	16.971	21.050	1.00	8.12	6
ATOM	2385	CA	PHE A 290						
ATOM	2386	CB	PHE A 290						
ATOM	2387	CG	PHE A 290						
ATOM	2388	CD	PHE A 290						
ATOM	2389	CE	PHE A 290						
ATOM	2390	CE1	PHE A 290						
ATOM	2391	CE2	PHE A 290						
ATOM	2392	CZ	PHE A 290						
ATOM	2393	C	PHE A 290						
ATOM	2394	O	PHE A 290						
ATOM	2395	N	ASN A 291						
ATOM	2396	CA	ASN A 291						
ATOM	2397	CB	ASN A 291						
ATOM	2398	CG	ASN A 291						
ATOM	2399	CD	ASN A 291						
ATOM	2400	CE	ASN A 291						
ATOM	2401	C	ASN A 291						
ATOM	2402	O	ASN A 291						
ATOM	2403	N	LEU A 292						
ATOM	2404	CA	LEU A 292						
ATOM	2405	CB	LEU A 292						
ATOM	2406	CG	LEU A 292						
ATOM	2407	CD	LEU A 292						
ATOM	2408	CE	LEU A 292						
ATOM	2409	C	LEU A 292						
ATOM	2410	N	GLN A 293						
ATOM	2411	CA	GLN A 293						
ATOM	2412	CB	GLN A 293						
ATOM	2413	CG	GLN A 293						
ATOM	2414	CD	GLN A 293						
ATOM	2415	CE	GLN A 293						
ATOM	2416	OE1	GLN A 293						
ATOM	2417	OE2	GLN A 293						
ATOM	2418	C	GLN A 293						
ATOM	2419	O	GLN A 293						
ATOM	2420	N	ALA A 294						
ATOM	2421	CA	ALA A 294						
ATOM	2422	CB	ALA A 294						
ATOM	2423	C	ALA A 294						
ATOM	2424	O	ALA A 294						
ATOM	2425	N	ALA A 295						
ATOM	2426	CA	ALA A 295						
ATOM	2427	CB	ALA A 295						
ATOM	2428	C	ALA A 295						
ATOM	2429	O	ALA A 295						
ATOM	2430	N	SER A 296						
ATOM	2431	CA	SER A 296						
ATOM	2432	CB	SER A 296						
ATOM	2433	CG	SER A 296						
ATOM	2434	C	SER A 296						
ATOM	2435	O	SER A 296						
ATOM	2436	N	SER A 297						
ATOM	2437	CA	SER A 297						
ATOM	2438	CB	SER A 297						

ATOM	2439	OG	SER A 297	42.921	18.303	13.176	1.00	20.24	8
ATOM	2440	C	SER A 297	42.921	16.146	10.508	1.00	15.90	6
ATOM	2441	O	SER A 297	44.076	16.216	10.160	1.00	15.87	6
ATOM	2442	N	GLN A 298	42.143	15.074	10.370	1.00	16.33	7
ATOM	2443	CA	GLN A 298	42.650	13.888	9.722	1.00	16.82	6
ATOM	2444	CB	GLN A 298	42.156	12.653	10.523	1.00	18.92	6
ATOM	2445	CG	GLN A 298	43.084	12.447	11.693	1.00	20.51	6
ATOM	2446	CD	GLN A 298	42.613	11.548	12.798	1.00	23.02	6
ATOM	2447	OE1	GLN A 298	42.174	10.410	12.588	1.00	24.09	8
ATOM	2448	NE2	GLN A 298	42.715	12.077	14.034	1.00	23.74	7
ATOM	2449	C	GLN A 298	42.319	13.823	8.245	1.00	17.02	6
ATOM	2450	O	GLN A 298	42.486	12.719	7.679	1.00	17.29	8
ATOM	2451	N	GLY A 299	41.907	14.913	7.631	1.00	16.90	7
ATOM	2452	CA	GLY A 299	41.595	15.001	6.223	1.00	16.90	6
ATOM	2453	C	GLY A 299	40.763	13.864	5.685	1.00	16.77	6
ATOM	2454	O	GLY A 299	40.942	13.480	4.523	1.00	17.33	8
ATOM	2455	N	GLY A 300	39.855	13.274	5.983	1.00	15.25	6
ATOM	2456	CA	GLY A 300	39.068	12.163	5.983	1.00	15.25	6
ATOM	2457	C	GLY A 300	39.483	10.868	6.650	1.00	14.82	6
ATOM	2458	O	GLY A 300	38.603	10.027	6.489	1.00	14.53	8
ATOM	2459	N	GLY A 301	40.574	10.532	7.302	1.00	14.47	7
ATOM	2460	CA	GLY A 301	40.815	9.227	7.860	1.00	14.37	6
ATOM	2461	C	GLY A 301	40.234	8.948	9.225	1.00	14.36	6
ATOM	2462	O	GLY A 301	40.318	7.830	9.696	1.00	14.17	8
ATOM	2463	N	TYR A 302	39.559	9.888	9.908	1.00	14.62	7
ATOM	2464	CA	TYR A 302	38.973	9.650	11.220	1.00	14.57	6
ATOM	2465	CB	TYR A 302	38.419	10.956	11.845	1.00	14.59	6
ATOM	2466	CG	TYR A 302	37.750	10.869	13.198	1.00	14.61	6
ATOM	2467	CD1	TYR A 302	38.559	10.860	14.355	1.00	14.96	6
ATOM	2468	CE1	TYR A 302	37.990	10.754	15.630	1.00	14.98	6
ATOM	2469	CD2	TYR A 302	36.380	10.751	13.400	1.00	14.40	6
ATOM	2470	CE2	TYR A 302	35.820	10.629	14.663	1.00	14.56	6
ATOM	2471	CZ	TYR A 302	36.622	10.655	15.778	1.00	14.83	6
ATOM	2472	OH	TYR A 302	36.157	10.564	17.049	1.00	15.01	8
ATOM	2473	C	TYR A 302	37.831	8.643	11.151	1.00	14.74	6
ATOM	2474	O	TYR A 302	37.073	8.682	10.170	1.00	14.62	8
ATOM	2475	N	ASP A 303	37.515	7.744	12.058	1.00	14.71	7
ATOM	2476	CA	ASP A 303	36.617	6.873	11.910	1.00	14.90	6
ATOM	2477	CB	ASP A 303	35.526	5.550	12.620	1.00	16.31	6
ATOM	2478	CG	ASP A 303	35.526	4.517	12.403	1.00	17.88	6
ATOM	2479	CD1	ASP A 303	34.383	4.796	12.005	1.00	17.07	8
ATOM	2480	CD2	ASP A 303	35.893	3.348	12.637	1.00	19.55	8
ATOM	2481	C	ASP A 303	35.165	7.627	12.500	1.00	14.85	8
ATOM	2482	O	ASP A 303	35.013	7.729	13.714	1.00	14.59	8
ATOM	2483	N	MET A 304	34.315	8.199	11.658	1.00	14.94	7
ATOM	2484	CA	MET A 304	33.151	8.973	12.057	1.00	15.29	6
ATOM	2485	CB	MET A 304	32.440	9.630	10.862	1.00	14.35	6
ATOM	2486	CG	MET A 304	33.307	10.718	10.201	1.00	13.91	6
ATOM	2487	SD	MET A 304	33.391	12.309	11.028	1.00	14.76	16
ATOM	2488	CE	MET A 304	31.941	13.156	10.378	1.00	11.94	6
ATOM	2489	C	MET A 304	32.161	8.195	10.378	1.00	11.94	6
ATOM	2490	O	MET A 304	31.322	8.846	13.549	1.00	15.60	6
ATOM	2491	N	ARG A 305	32.251	6.872	13.019	1.00	15.77	7
ATOM	2492	CA	ARG A 305	31.372	6.123	13.883	1.00	16.15	6
ATOM	2493	CB	ARG A 305	31.398	4.601	13.558	1.00	17.94	6
ATOM	2494	CG	ARG A 305	30.683	4.270	12.266	1.00	20.53	6
ATOM	2495	CD	ARG A 305	30.984	3.018	11.512	1.00	21.54	6
ATOM	2496	NE	ARG A 305	32.390	2.813	11.326	1.00	23.87	7
ATOM	2497	CZ	ARG A 305	32.917	1.717	10.819	1.00	26.93	6
ATOM	2498	NH1	ARG A 305	32.145	0.716	10.412	1.00	29.01	7
ATOM	2499	NH2	ARG A 305	34.239	1.652	10.753	1.00	28.19	7
ATOM	2500	C	ARG A 305	31.768	5.318	15.354	1.00	16.33	6
ATOM	2501	O	ARG A 305	30.997	5.924	16.218	1.00	16.15	8
ATOM	2502	N	LYS A 306	32.942	6.837	15.661	1.00	16.51	7
ATOM	2503	CA	LYS A 306	33.424	7.006	17.011	1.00	17.04	6
ATOM	2504	CB	LYS A 306	34.945	6.643	16.903	1.00	17.04	6
ATOM	2505	CG	LYS A 306	35.043	5.174	16.504	1.00	25.08	6
ATOM	2506	CD	LYS A 306	36.487	4.726	16.705	1.00	30.20	6
ATOM	2507	CE	LYS A 306	36.968	3.663	15.712	1.00	32.87	6
ATOM	2508	NZ	LYS A 306	37.911	2.695	16.442	1.00	35.11	7
ATOM	2509	C	LYS A 306	33.356	8.375	17.653	1.00	17.07	6
ATOM	2510	O	LYS A 306	33.967	8.639	18.692	1.00	16.98	8
ATOM	2511	N	LEU A 307	32.639	9.313	17.026	1.00	17.11	7
ATOM	2512	CA	LEU A 307	32.539	10.700	17.444	1.00	17.21	6
ATOM	2513	CB	LEU A 307	31.688	11.509	16.526	1.00	18.35	6
ATOM	2514	CG	LEU A 307	32.192	12.263	15.348	1.00	20.88	6
ATOM	2515	CD1	LEU A 307	31.055	12.963	14.582	1.00	21.03	6
ATOM	2516	CD2	LEU A 307	33.273	13.283	15.684	1.00	20.35	6
ATOM	2517	C	LEU A 307	32.084	10.626	18.890	1.00	17.01	6
ATOM	2518	O	LEU A 307	32.553	11.677	19.605	1.00	17.09	8
ATOM	2519	N	LEU A 308	31.179	9.970	19.331	1.00	16.89	7
ATOM	2520	CA	LEU A 308	30.629	9.973	20.670	1.00	16.75	6
ATOM	2521	CB	LEU A 308	29.153	9.440	20.589	1.00	17.24	6
ATOM	2522	CG	LEU A 308	28.116	10.476	20.136	1.00	19.15	6
ATOM	2523	CD1	LEU A 308	28.740	9.862	19.977	1.00	18.81	6
ATOM	2524	CD2	LEU A 308	28.015	11.685	21.063	1.00	19.79	6
ATOM	2525	C	LEU A 308	31.420	9.200	21.720	1.00	16.38	6
ATOM	2526	O	LEU A 308	31.137	9.327	22.922	1.00	16.30	8
ATOM	2527	N	ASN A 309	32.381	8.386	21.344	1.00	16.16	7
ATOM	2528	CA	ASN A 309	33.203	7.595	22.228	1.00	15.89	6
ATOM	2529	CB	ASN A 309	34.349	6.886	21.692	1.00	21.07	6
ATOM	2530	CG	ASN A 309	33.880	5.720	20.660	1.00	26.35	6
ATOM	2531	CD1	ASN A 309	34.746	5.049	20.024	1.00	29.82	8
ATOM	2532	CD2	ASN A 309	32.579	5.435	20.588	1.00	27.51	7
ATOM	2533	C	ASN A 309	33.938	8.456	23.265	1.00	15.16	6
ATOM	2534	O	ASN A 309	34.623	9.384	22.831	1.00	15.00	8
ATOM	2535	N	GLY A 310	33.777	8.102	24.545	1.00	14.32	7
ATOM	2536	CA	GLY A 310	34.447	8.836	25.603	1.00	13.49	6
ATOM	2537	C	GLY A 310	33.944	10.232	25.938	1.00	12.69	6
ATOM	2538	O	GLY A 310	34.647	10.890	26.657	1.00	12.41	8
ATOM	2539	N	THR A 311	32.784	10.615	25.413	1.00	12.19	7
ATOM	2540	CA	THR A 311	32.222	11.929	25.676	1.00	11.65	6
ATOM	2541	CB	THR A 311	31.462	12.519	24.452	1.00	10.26	6
ATOM	2542	CG1	THR A 311	30.315	11.692	24.240	1.00	10.86	8
ATOM	2543	CG2	THR A 311	32.307	12.571	23.191	1.00	8.42	6
ATOM	2544	C	THR A 311	31.284	11.908	26.895	1.00	11.36	6

ATOM	2545	O	THR A 311	30.667	10.902	27.258	1.00	11.29	8
ATOM	2546	N	VAL A 312	31.198	13.075	27.545	1.00	11.20	7
ATOM	2547	CA	VAL A 312	30.313	13.282	28.693	1.00	11.29	6
ATOM	2548	CB	VAL A 312	30.567	14.637	29.407	1.00	12.62	6
ATOM	2549	CG1	VAL A 312	29.620	14.906	30.597	1.00	13.45	6
ATOM	2550	CG2	VAL A 312	31.995	14.730	29.912	1.00	10.56	6
ATOM	2551	C	VAL A 312	28.874	13.189	28.191	1.00	11.23	6
ATOM	2552	O	VAL A 312	28.053	12.526	28.793	1.00	11.01	8
ATOM	2553	N	VAL A 313	28.533	13.825	27.061	1.00	11.42	7
ATOM	2554	CA	VAL A 313	27.208	13.790	26.498	1.00	11.94	6
ATOM	2555	CB	VAL A 313	27.107	14.723	25.266	1.00	12.88	6
ATOM	2556	CG1	VAL A 313	27.604	14.175	23.942	1.00	13.11	6
ATOM	2557	CG2	VAL A 313	25.627	15.102	25.100	1.00	14.06	6
ATOM	2558	C	VAL A 313	26.655	12.380	26.219	1.00	12.21	6
ATOM	2559	O	VAL A 314	25.434	12.216	26.319	1.00	11.69	8
ATOM	2560	N	SER A 314	27.418	11.313	25.971	1.00	12.83	7
ATOM	2561	CA	SER A 314	26.878	9.987	25.750	1.00	13.56	6
ATOM	2562	CB	SER A 314	27.801	9.054	24.922	1.00	13.63	6
ATOM	2563	CG	SER A 314	29.056	9.048	25.641	1.00	15.90	8
ATOM	2564	C	SER A 314	26.572	9.365	27.111	1.00	14.04	6
ATOM	2565	O	SER A 314	25.730	8.445	27.105	1.00	14.28	8
ATOM	2566	N	LVS A 315	27.168	9.725	28.254	1.00	14.23	7
ATOM	2567	CA	LVS A 315	26.823	9.081	29.513	1.00	19.81	6
ATOM	2568	CB	LVS A 315	27.928	8.797	30.491	1.00	14.22	6
ATOM	2569	CG	LVS A 315	29.333	8.495	30.319	1.00	26.75	6
ATOM	2570	CE	LVS A 315	30.321	9.661	30.402	1.00	32.69	6
ATOM	2571	CD	LVS A 315	30.714	10.114	31.825	1.00	35.30	6
ATOM	2572	HZ	LVS A 315	31.599	9.199	32.634	1.00	35.57	7
ATOM	2573	C	LVS A 315	25.884	9.951	30.379	1.00	13.74	6
ATOM	2574	O	LVS A 315	26.969	9.435	31.020	1.00	13.60	8
ATOM	2575	N	HIS A 316	26.108	11.257	30.397	1.00	13.12	7
ATOM	2576	CA	HIS A 316	25.314	12.197	31.179	1.00	13.02	6
ATOM	2577	CB	HIS A 316	26.202	12.791	32.327	1.00	12.69	6
ATOM	2578	CG	HIS A 316	26.550	11.718	33.313	1.00	12.94	6
ATOM	2579	CD2	HIS A 316	25.796	11.024	34.166	1.00	13.25	6
ATOM	2580	HD1	HIS A 316	27.835	11.194	33.424	1.00	15.42	7
ATOM	2581	CE1	HIS A 316	27.850	10.206	34.317	1.00	14.97	6
ATOM	2582	HE2	HIS A 316	26.617	10.106	34.822	1.00	15.47	7
ATOM	2583	C	HIS A 316	24.809	13.360	30.325	1.00	12.64	6
ATOM	2584	O	HIS A 316	25.304	14.479	30.471	1.00	12.29	8
ATOM	2585	N	PRO A 317	23.868	13.075	29.435	1.00	12.52	7
ATOM	2586	CD	PRO A 317	23.256	11.740	29.268	1.00	12.43	6
ATOM	2587	CA	PRO A 317	23.311	14.040	28.519	1.00	12.50	6
ATOM	2588	CB	PRO A 317	22.280	13.268	27.640	1.00	12.54	6
ATOM	2589	CG	PRO A 317	21.996	12.051	28.524	1.00	12.55	6
ATOM	2590	C	PRO A 317	22.669	15.253	29.133	1.00	12.59	6
ATOM	2591	O	PRO A 317	22.750	16.369	28.542	1.00	12.68	8
ATOM	2592	N	LEU A 318	22.033	15.168	30.285	1.00	12.44	7
ATOM	2593	CA	LEU A 318	21.370	16.286	30.956	1.00	12.38	6
ATOM	2594	CB	LEU A 318	20.278	15.805	31.970	1.00	13.77	6
ATOM	2595	CG	LEU A 318	19.256	14.834	31.334	1.00	15.85	6
ATOM	2596	CD1	LEU A 318	18.250	14.143	32.241	1.00	15.19	6
ATOM	2597	CD2	LEU A 318	18.520	15.629	30.254	1.00	17.19	6
ATOM	2598	C	LEU A 318	17.175	31.741	17.175	1.00	11.91	6
ATOM	2599	O	LEU A 318	21.929	18.174	32.286	1.00	11.51	8
ATOM	2600	N	LVS A 319	23.402	16.757	31.836	1.00	11.53	7
ATOM	2601	CA	LVS A 319	24.559	17.559	32.591	1.00	11.24	6
ATOM	2602	CB	LVS A 319	25.135	16.758	33.794	1.00	12.25	6
ATOM	2603	CG	LVS A 319	24.001	16.369	34.812	1.00	12.23	6
ATOM	2604	CD	LVS A 319	23.655	17.705	35.470	1.00	13.91	6
ATOM	2605	CE	LVS A 319	22.335	17.774	36.181	1.00	15.19	6
ATOM	2606	HZ	LVS A 319	22.278	18.963	37.119	1.00	14.09	7
ATOM	2607	C	LVS A 319	25.652	18.008	31.640	1.00	10.89	6
ATOM	2608	O	LVS A 319	26.717	18.376	32.153	1.00	11.10	8
ATOM	2609	N	SER A 320	26.564	18.409	29.483	1.00	10.24	7
ATOM	2610	CA	SER A 320	26.542	17.969	30.320	1.00	9.74	6
ATOM	2611	CB	SER A 320	26.825	17.443	28.311	1.00	11.44	6
ATOM	2612	CG	SER A 320	26.960	16.158	28.752	1.00	15.00	8
ATOM	2613	C	SER A 320	26.322	19.681	28.692	1.00	9.08	6
ATOM	2614	O	SER A 320	25.215	19.672	28.144	1.00	9.21	8
ATOM	2615	N	VAL A 321	27.294	20.549	28.581	1.00	8.35	7
ATOM	2616	CA	VAL A 321	27.166	21.744	27.760	1.00	7.87	6
ATOM	2617	CB	VAL A 321	27.455	23.085	28.447	1.00	6.55	6
ATOM	2618	CG1	VAL A 321	27.468	24.283	27.473	1.00	5.70	6
ATOM	2619	CG2	VAL A 321	26.352	23.381	29.489	1.00	6.25	6
ATOM	2620	C	VAL A 321	28.079	21.422	26.585	1.00	7.79	6
ATOM	2621	O	VAL A 321	29.282	21.146	26.791	1.00	8.06	8
ATOM	2622	N	THR A 322	27.497	21.399	25.396	1.00	7.46	7
ATOM	2623	CA	THR A 322	28.302	21.038	24.183	1.00	7.12	6
ATOM	2624	CB	THR A 322	27.504	20.146	23.199	1.00	5.50	8
ATOM	2625	CG1	THR A 322	26.184	20.559	22.923	1.00	5.00	6
ATOM	2626	CG2	THR A 322	27.279	18.718	23.807	1.00	6.18	6
ATOM	2627	C	THR A 322	28.877	22.262	23.492	1.00	7.07	6
ATOM	2628	O	THR A 322	28.206	23.319	23.510	1.00	7.34	8
ATOM	2629	N	PHE A 323	30.076	22.181	22.907	1.00	6.79	7
ATOM	2630	CA	PHE A 323	30.734	23.301	22.257	1.00	6.58	6
ATOM	2631	CB	PHE A 323	31.435	24.192	23.312	1.00	5.72	6
ATOM	2632	CG	PHE A 323	32.752	23.783	23.849	1.00	5.21	6
ATOM	2633	CD1	PHE A 323	33.918	24.279	23.270	1.00	6.61	6
ATOM	2634	CD2	PHE A 323	32.864	22.861	24.884	1.00	6.77	6
ATOM	2635	CE1	PHE A 323	35.167	23.880	23.764	1.00	7.34	6
ATOM	2636	CE2	PHE A 323	34.105	22.368	25.363	1.00	6.08	6
ATOM	2637	CZ	PHE A 323	35.238	22.944	24.795	1.00	6.00	6
ATOM	2638	C	PHE A 323	31.727	22.855	21.184	1.00	6.75	6
ATOM	2639	O	PHE A 323	32.313	21.743	21.207	1.00	6.74	8
ATOM	2640	N	VAL A 324	31.917	23.744	20.208	1.00	6.84	7
ATOM	2641	CA	VAL A 324	32.846	23.539	19.087	1.00	6.92	6
ATOM	2642	CB	VAL A 324	32.248	24.084	17.759	1.00	6.12	6
ATOM	2643	CG1	VAL A 324	33.175	23.923	16.595	1.00	5.00	6
ATOM	2644	CG2	VAL A 324	30.945	23.335	17.428	1.00	5.00	6
ATOM	2645	C	VAL A 324	34.230	24.137	19.434	1.00	7.23	6
ATOM	2646	O	VAL A 324	35.247	23.410	19.508	1.00	6.91	8
ATOM	2647	N	ASP A 325	34.276	25.479	19.678	1.00	7.39	7
ATOM	2648	CA	ASP A 325	35.469	26.189	20.078	1.00	7.78	6
ATOM	2649	CB	ASP A 325	36.180	26.898	18.918	1.00	8.62	6
ATOM	2650	CG	ASP A 325	37.157	25.954	18.192	1.00	8.81	6

SUBSTITUTE SHEET (RULE 26)

2651	ATOM	001 ASP A 325	38.076	25.409	18.839	1.00	7.66	8	ATOM	2704	N	GLY A 332	46.122	30.893	18.593	1.00	15.77	7
2652	ATOM	002 ASP A 325	37.027	25.482	16.966	1.00	9.34	8	ATOM	2705	CA	GLY A 332	47.087	31.624	19.404	1.00	17.06	6
2653	ATOM	003 ASP A 325	35.117	27.261	21.116	1.00	8.18	6	ATOM	2706	C	GLY A 332	46.881	31.463	20.896	1.00	18.22	6
2654	ATOM	004 ASP A 325	33.960	27.635	21.254	1.00	8.16	8	ATOM	2707	O	GLY A 332	47.755	31.915	21.633	1.00	18.26	8
2655	ATOM	005 ASN A 326	36.108	27.788	21.826	1.00	8.35	7	ATOM	2708	N	GLM A 333	45.817	30.862	21.429	1.00	19.06	7
2656	ATOM	006 ASN A 326	35.925	28.845	22.813	1.00	8.28	6	ATOM	2709	CA	GLM A 333	45.678	30.778	22.875	1.00	19.08	6
2657	ATOM	007 ASN A 326	35.487	28.329	22.160	1.00	9.54	6	ATOM	2710	CB	GLM A 333	44.181	30.838	23.241	1.00	19.70	6
2658	ATOM	008 ASN A 326	36.502	27.485	24.902	1.00	11.91	6	ATOM	2711	CG	GLM A 333	43.711	32.283	23.072	1.00	20.78	6
2659	ATOM	009 ASN A 326	37.701	27.415	24.622	1.00	12.52	8	ATOM	2712	CD	GLM A 333	44.572	33.254	23.876	1.00	23.47	6
2660	ATOM	010 ASN A 326	36.121	28.782	23.965	1.00	11.95	7	ATOM	2713	OE1	GLM A 333	45.181	34.191	23.315	1.00	26.12	8
2661	ATOM	011 ASN A 326	37.212	29.685	22.871	1.00	8.44	6	ATOM	2714	ME2	GLM A 333	44.705	33.056	25.175	1.00	22.30	7
2662	ATOM	012 ASN A 326	38.140	29.601	22.053	1.00	7.98	8	ATOM	2715	C	GLM A 333	46.462	29.622	23.446	1.00	20.87	6
2663	ATOM	013 HIS A 327	37.266	30.626	23.836	1.00	8.65	7	ATOM	2716	O	GLM A 333	47.167	28.850	22.773	1.00	20.84	8
2664	ATOM	014 HIS A 327	38.367	31.562	23.994	1.00	9.17	6	ATOM	2717	N	SER A 334	46.339	29.555	24.795	1.00	21.65	7
2665	ATOM	015 HIS A 327	37.976	32.718	24.999	1.00	8.48	6	ATOM	2718	CA	SER A 334	47.083	28.519	25.552	1.00	22.42	6
2666	ATOM	016 HIS A 327	37.800	32.154	26.392	1.00	7.81	6	ATOM	2719	CB	SER A 334	46.792	28.705	27.067	1.00	26.55	6
2667	ATOM	017 HIS A 327	38.481	32.357	27.535	1.00	7.34	6	ATOM	2720	OG	SER A 334	45.405	29.089	27.235	1.00	30.85	8
2668	ATOM	018 HIS A 327	36.785	31.222	26.672	1.00	7.98	6	ATOM	2721	O	SER A 334	46.790	27.074	25.194	1.00	22.23	6
2669	ATOM	019 HIS A 327	36.886	30.856	27.951	1.00	8.46	7	ATOM	2722	O	SER A 334	47.687	26.293	24.929	1.00	22.55	8
2670	ATOM	020 HIS A 327	37.883	31.338	28.493	1.00	8.30	7	ATOM	2723	N	LEU A 335	45.506	26.728	25.170	1.00	21.74	7
2671	ATOM	021 HIS A 327	39.664	30.866	24.406	1.00	9.58	6	ATOM	2724	CA	LEU A 335	44.958	25.411	24.863	1.00	20.75	6
2672	ATOM	022 HIS A 327	40.718	31.444	24.169	1.00	9.63	8	ATOM	2725	CB	LEU A 335	43.814	25.183	25.883	1.00	22.04	6
2673	ATOM	023 HIS A 327	39.645	29.653	24.928	1.00	10.01	7	ATOM	2726	CG	LEU A 335	44.252	25.266	27.365	1.00	23.70	6
2674	ATOM	024 ASP A 328	40.783	28.869	25.312	1.00	10.53	6	ATOM	2727	CD1	LEU A 335	43.065	25.292	28.305	1.00	23.07	6
2675	ATOM	025 ASP A 328	40.422	27.735	26.312	1.00	14.56	6	ATOM	2728	CD2	LEU A 335	45.184	24.089	27.673	1.00	24.51	6
2676	ATOM	026 ASP A 328	39.676	27.936	27.629	1.00	18.50	6	ATOM	2729	C	LEU A 335	44.460	25.313	23.427	1.00	19.68	6
2677	ATOM	027 ASP A 328	40.162	28.843	28.385	1.00	17.22	8	ATOM	2730	O	LEU A 335	43.491	24.609	23.136	1.00	19.77	8
2678	ATOM	028 ASP A 328	38.615	27.265	28.055	1.00	10.47	8	ATOM	2731	N	GLU A 336	45.111	26.053	22.536	1.00	18.47	7
2679	ATOM	029 ASP A 328	41.385	28.188	24.074	1.00	10.45	6	ATOM	2732	CA	GLU A 336	44.766	26.089	21.149	1.00	17.45	6
2680	ATOM	030 ASP A 328	42.687	28.841	23.933	1.00	10.58	8	ATOM	2733	CB	GLU A 336	45.908	26.773	20.387	1.00	19.49	6
2681	ATOM	031 THR A 329	40.518	27.688	23.167	1.00	10.47	7	ATOM	2734	CG	GLU A 336	45.655	26.544	18.905	1.00	22.99	6
2682	ATOM	032 THR A 329	40.946	26.880	22.028	1.00	10.37	6	ATOM	2735	CD	GLU A 336	46.508	27.440	18.036	1.00	26.38	6
2683	ATOM	033 THR A 329	39.933	25.709	21.777	1.00	10.26	6	ATOM	2736	OE1	GLU A 336	47.378	28.166	18.504	1.00	26.94	8
2684	ATOM	034 THR A 329	38.709	26.293	21.286	1.00	9.63	8	ATOM	2737	OE2	GLU A 336	46.276	27.487	16.805	1.00	28.18	8
2685	ATOM	035 THR A 329	39.596	24.873	23.020	1.00	9.29	6	ATOM	2738	C	GLU A 336	44.504	24.698	20.571	1.00	16.40	6
2686	ATOM	036 THR A 329	41.142	27.596	20.702	1.00	10.36	6	ATOM	2739	O	GLU A 336	45.349	23.802	20.647	1.00	16.09	8
2687	ATOM	037 THR A 329	41.563	26.999	19.704	1.00	9.94	8	ATOM	2740	N	SER A 337	43.338	24.527	19.954	1.00	15.33	7
2688	ATOM	038 GLW A 330	40.827	28.878	20.679	1.00	10.77	7	ATOM	2741	CA	SER A 337	43.005	23.217	19.393	1.00	14.23	6
2689	ATOM	039 GLW A 330	40.985	29.688	19.441	1.00	11.30	6	ATOM	2742	CB	SER A 337	42.891	22.175	20.487	1.00	13.48	6
2690	ATOM	040 GLW A 330	40.182	30.988	19.518	1.00	9.13	6	ATOM	2743	OG	SER A 337	41.855	22.515	21.439	1.00	13.96	8
2691	ATOM	041 GLW A 330	40.769	31.987	20.543	1.00	8.40	6	ATOM	2744	C	SER A 337	41.679	23.436	18.645	1.00	13.82	6
2692	ATOM	042 GLW A 330	40.003	33.322	20.559	1.00	8.40	6	ATOM	2745	O	SER A 337	40.615	22.864	18.896	1.00	13.37	8
2693	ATOM	043 GLW A 330	39.089	33.499	21.393	1.00	7.21	8	ATOM	2746	N	THR A 338	41.878	24.333	17.679	1.00	13.46	7
2694	ATOM	044 GLW A 330	40.432	34.237	19.660	1.00	7.16	7	ATOM	2747	CA	THR A 338	40.800	24.801	16.837	1.00	13.53	6
2695	ATOM	045 GLW A 330	42.486	29.890	19.211	1.00	11.99	6	ATOM	2748	CB	THR A 338	41.340	26.036	16.033	1.00	13.02	6
2696	ATOM	046 GLW A 330	43.345	29.690	20.092	1.00	11.70	8	ATOM	2749	OG1	THR A 338	41.955	26.893	17.006	1.00	14.55	8
2697	ATOM	047 PRO A 331	42.793	30.208	17.963	1.00	12.80	7	ATOM	2750	CG2	THR A 338	40.259	26.794	15.338	1.00	12.29	6
2698	ATOM	048 PRO A 331	41.806	30.403	16.873	1.00	12.95	6	ATOM	2751	C	THR A 338	40.216	23.770	15.877	1.00	13.20	6
2699	ATOM	049 PRO A 331	44.119	30.424	17.447	1.00	13.52	6	ATOM	2752	O	THR A 338	40.980	23.008	15.281	1.00	13.26	8
2700	ATOM	050 PRO A 331	43.974	30.918	15.966	1.00	13.53	6	ATOM	2753	N	VAL A 339	38.905	23.766	15.743	1.00	12.73	7
2701	ATOM	051 PRO A 331	42.608	30.336	15.583	1.00	13.10	6	ATOM	2754	CA	VAL A 339	38.270	22.857	14.783	1.00	12.66	6
2702	ATOM	052 PRO A 331	44.899	31.372	18.320	1.00	14.55	6	ATOM	2755	CB	VAL A 339	36.803	22.594	15.154	1.00	11.55	6
2703	ATOM	053 PRO A 331	44.496	32.463	18.767	1.00	14.46	8	ATOM	2756	CG1	VAL A 339	36.030	21.874	14.057	1.00	9.87	6

SUBSTITUTE SHEET (RULE 26)

ATOM	2757	CG2	VAL	A	339	36.745	21.811	16.483	1.00	9.266	6	7
ATOM	2758	C	VAL	A	339	38.513	23.484	13.365	1.00	12.57	6	6
ATOM	2759	O	VAL	A	339	38.271	24.688	13.279	1.00	12.26	8	6
ATOM	2760	N	GLM	A	340	39.016	22.686	12.404	1.00	12.55	7	6
ATOM	2761	CA	GLM	A	340	39.280	23.302	11.088	1.00	12.55	6	6
ATOM	2762	CB	GLM	A	340	39.975	22.357	10.097	1.00	11.11	6	6
ATOM	2763	CG	GLM	A	340	41.372	21.974	10.559	1.00	11.55	6	6
ATOM	2764	CD	GLM	A	340	42.073	21.105	9.513	1.00	14.34	6	6
ATOM	2765	OE1	GLM	A	340	41.594	20.802	8.384	1.00	15.11	8	6
ATOM	2766	NE2	GLM	A	340	43.272	20.743	9.959	1.00	12.61	7	6
ATOM	2767	C	GLM	A	340	38.009	23.900	10.468	1.00	12.34	6	6
ATOM	2768	O	GLM	A	340	36.930	23.331	10.565	1.00	12.28	8	6
ATOM	2769	N	THR	A	341	38.167	23.042	9.779	1.00	12.25	7	6
ATOM	2770	CA	THR	A	341	37.024	25.755	9.200	1.00	12.38	6	6
ATOM	2771	CB	THR	A	341	37.516	26.993	8.393	1.00	15.06	6	6
ATOM	2772	CG1	THR	A	341	38.100	27.874	9.353	1.00	16.92	8	6
ATOM	2773	CG2	THR	A	341	36.347	27.684	7.716	1.00	14.77	6	6
ATOM	2774	C	THR	A	341	36.124	24.916	8.332	1.00	12.08	6	6
ATOM	2775	O	THR	A	341	34.910	25.018	8.411	1.00	12.16	8	6
ATOM	2776	N	TRP	A	342	36.698	24.095	7.465	1.00	11.85	7	6
ATOM	2777	CA	TRP	A	342	35.902	23.225	6.585	1.00	11.19	6	6
ATOM	2778	CB	TRP	A	342	36.871	22.438	5.673	1.00	10.89	6	6
ATOM	2779	CG	TRP	A	342	37.568	21.288	6.392	1.00	9.86	6	6
ATOM	2780	CD2	TRP	A	342	37.988	19.219	6.491	1.00	9.37	6	6
ATOM	2781	CE1	TRP	A	342	35.916	19.290	5.991	1.00	10.12	6	6
ATOM	2782	CE3	TRP	A	342	38.756	21.330	7.062	1.00	10.06	6	6
ATOM	2783	NE1	TRP	A	342	39.027	20.080	7.592	1.00	11.11	7	6
ATOM	2784	NE2	TRP	A	342	37.809	17.853	7.527	1.00	10.50	6	6
ATOM	2785	C22	TRP	A	342	35.700	17.950	6.293	1.00	10.34	6	6
ATOM	2786	CH2	TRP	A	342	36.654	17.222	7.050	1.00	10.76	6	6
ATOM	2787	C	TRP	A	342	34.988	22.340	7.391	1.00	10.76	6	6
ATOM	2788	O	TRP	A	342	33.837	22.038	6.990	1.00	10.60	8	6
ATOM	2789	N	PHE	A	343	35.375	21.846	8.577	1.00	10.45	7	6
ATOM	2790	CA	PHE	A	343	36.544	20.979	9.389	1.00	9.81	6	6
ATOM	2791	CB	PHE	A	343	35.520	20.088	10.193	1.00	10.59	6	6
ATOM	2792	CB	PHE	A	343	34.561	17.786	9.989	1.00	9.97	6	6
ATOM	2793	CG	PHE	A	343	36.861	18.880	10.796	1.00	9.94	6	6
ATOM	2794	CD1	PHE	A	343	34.466	18.875	12.117	1.00	9.30	6	6
ATOM	2795	CD2	PHE	A	343	33.947	16.653	10.504	1.00	9.66	6	6
ATOM	2796	CE1	PHE	A	343	33.862	17.747	12.659	1.00	10.16	6	6
ATOM	2797	CE2	PHE	A	343	33.592	16.637	11.845	1.00	10.55	6	6
ATOM	2798	CZ	PHE	A	343	33.621	21.720	10.332	1.00	9.65	6	6
ATOM	2799	C	PHE	A	343	33.897	23.010	10.569	1.00	9.52	7	6
ATOM	2800	O	PHE	A	343	32.649	21.140	10.826	1.00	9.50	8	6
ATOM	2801	N	LYS	A	344	33.084	23.775	11.536	1.00	11.03	6	6
ATOM	2802	CA	LYS	A	344	33.689	25.209	11.614	1.00	11.03	6	6
ATOM	2803	CB	LYS	A	344	33.193	25.978	12.846	1.00	11.47	6	6
ATOM	2804	CG	LYS	A	344	34.235	26.954	13.366	1.00	10.60	6	6
ATOM	2805	CD	LYS	A	344	36.068	26.281	14.470	1.00	9.19	7	6
ATOM	2806	CE	LYS	A	344	36.098	27.262	14.962	1.00	7.52	6	6
ATOM	2807	CZ	LYS	A	344	31.573	23.696	11.384	1.00	9.62	6	6
ATOM	2808	C	LYS	A	344	30.838	23.428	12.371	1.00	9.63	8	6
ATOM	2809	O	LYS	A	344							
ATOM	2810	N	PRO	A	345	30.989	23.886	10.213	1.00	9.37	7	6
ATOM	2811	CD	PRO	A	345	31.697	24.236	8.991	1.00	9.33	6	6
ATOM	2812	CA	PRO	A	345	29.559	23.779	10.018	1.00	9.01	6	6
ATOM	2813	CB	PRO	A	345	29.285	26.265	8.592	1.00	9.17	6	6
ATOM	2814	CG	PRO	A	345	30.576	25.000	8.288	1.00	9.42	6	6
ATOM	2815	C	PRO	A	345	29.077	22.331	10.309	1.00	8.68	6	6
ATOM	2816	O	PRO	A	345	27.992	22.162	10.862	1.00	8.28	8	6
ATOM	2817	N	LEU	A	346	29.863	21.274	9.998	1.00	8.29	7	6
ATOM	2818	CA	LEU	A	346	29.491	19.890	10.274	1.00	7.82	6	6
ATOM	2819	CB	LEU	A	346	30.443	18.876	9.644	1.00	7.71	6	6
ATOM	2820	CG	LEU	A	346	30.608	18.730	8.147	1.00	9.48	6	6
ATOM	2821	CD1	LEU	A	346	30.910	20.053	7.472	1.00	9.58	6	6
ATOM	2822	CD2	LEU	A	346	31.710	17.710	7.794	1.00	9.58	6	6
ATOM	2823	C	LEU	A	346	29.426	19.714	11.796	1.00	7.55	6	6
ATOM	2824	O	LEU	A	346	28.510	19.084	12.262	1.00	7.43	8	6
ATOM	2825	N	ALA	A	347	30.320	20.297	12.583	1.00	7.30	7	6
ATOM	2826	CA	ALA	A	347	30.425	20.274	14.019	1.00	7.11	6	6
ATOM	2827	CB	ALA	A	347	31.740	20.902	14.501	1.00	7.21	6	6
ATOM	2828	C	ALA	A	347	29.264	21.031	14.671	1.00	7.06	6	6
ATOM	2829	N	TYR	A	348	28.712	20.558	15.670	1.00	7.03	8	6
ATOM	2830	CA	TYR	A	348	28.827	22.160	14.103	1.00	7.17	7	6
ATOM	2831	CB	TYR	A	348	27.673	22.854	14.693	1.00	7.45	6	6
ATOM	2832	CG	TYR	A	348	27.650	24.299	14.175	1.00	7.45	6	6
ATOM	2833	CD1	TYR	A	348	28.510	25.236	15.008	1.00	7.77	6	6
ATOM	2834	CE1	TYR	A	348	29.718	25.772	14.609	1.00	7.85	6	6
ATOM	2835	CE2	TYR	A	348	30.416	26.670	15.415	1.00	7.87	6	6
ATOM	2836	CE3	TYR	A	348	28.035	25.569	16.285	1.00	7.82	6	6
ATOM	2837	CZ	TYR	A	348	28.731	26.430	17.105	1.00	7.89	6	6
ATOM	2838	O	TYR	A	348	29.917	26.984	16.682	1.00	7.94	6	6
ATOM	2839	N	TRP	A	348	30.609	27.789	17.576	1.00	7.87	8	6
ATOM	2840	C	TRP	A	348	26.404	22.081	14.387	1.00	7.12	6	6
ATOM	2841	O	ALA	A	349	25.461	22.029	15.193	1.00	7.05	8	6
ATOM	2842	N	ALA	A	349	26.328	21.385	13.223	1.00	6.87	7	6
ATOM	2843	CA	ALA	A	349	25.127	20.607	12.939	1.00	6.67	6	6
ATOM	2844	CB	ALA	A	349	25.131	20.070	11.515	1.00	6.51	6	6
ATOM	2845	C	ALA	A	349	25.054	19.497	13.978	1.00	6.62	6	6
ATOM	2846	O	ALA	A	349	23.995	19.114	14.487	1.00	6.43	8	6
ATOM	2847	N	PHE	A	350	26.237	18.899	14.250	1.00	6.67	7	6
ATOM	2848	CA	PHE	A	350	26.268	17.814	15.220	1.00	6.81	6	6
ATOM	2849	CB	PHE	A	350	27.701	17.250	15.304	1.00	6.91	6	6
ATOM	2850	CG	PHE	A	350	27.766	15.996	16.137	1.00	9.15	6	6
ATOM	2851	CD1	PHE	A	350	27.494	14.763	15.559	1.00	8.95	6	6
ATOM	2852	CD2	PHE	A	350	28.009	16.069	17.510	1.00	11.23	6	6
ATOM	2853	CE1	PHE	A	350	27.551	13.618	16.317	1.00	10.89	6	6
ATOM	2854	CE2	PHE	A	350	28.044	14.894	18.273	1.00	11.66	6	6
ATOM	2855	CZ	PHE	A	350	27.847	13.657	17.687	1.00	10.74	6	6
ATOM	2856	C	PHE	A	350	25.768	18.242	16.605	1.00	6.90	6	6
ATOM	2857	O	PHE	A	350	24.978	17.547	17.275	1.00	6.86	8	6
ATOM	2858	N	ILE	A	351	26.217	19.408	17.102	1.00	7.14	7	6
ATOM	2859	CA	ILE	A	351	25.736	19.797	18.437	1.00	7.28	6	6
ATOM	2860	CB	ILE	A	351	26.767	20.463	19.194	1.00	6.43	6	6
ATOM	2861	CG	ILE	A	351	28.084	19.924	19.275	1.00	6.52	6	6
ATOM	2862	CG1	ILE	A	351	26.943	22.024	18.556	1.00	6.43	6	6

ATOM	2863	CD1	ILE	A	351	27.589	22.986	19.575	1.00	5.33	6	ATOM	2916	CE1	TYR	A	358	21.449	26.080	26.747	1.00	9.42	6
ATOM	2864	C	ILE	A	351	24.372	20.509	18.459	1.00	7.26	6	ATOM	2917	CD2	TYR	A	358	22.294	24.466	28.799	1.00	9.67	6
ATOM	2865	O	ILE	A	351	23.668	20.349	19.498	1.00	7.46	8	ATOM	2918	CE2	TYR	A	358	21.900	25.783	29.085	1.00	9.55	6
ATOM	2866	N	LEU	A	352	23.960	21.213	17.423	1.00	7.13	7	ATOM	2919	CZ	TYR	A	358	21.466	26.587	28.050	1.00	9.41	6
ATOM	2867	CA	LEU	A	352	22.678	21.931	17.500	1.00	7.51	6	ATOM	2920	OH	TYR	A	358	21.076	27.879	28.304	1.00	8.90	8
ATOM	2868	CB	LEU	A	352	22.778	23.170	16.614	1.00	6.11	6	ATOM	2921	C	TYR	A	358	24.062	22.642	25.113	1.00	9.49	6
ATOM	2869	CG	LEU	A	352	23.789	24.248	17.000	1.00	7.70	6	ATOM	2922	O	TYR	A	358	25.195	22.737	25.552	1.00	9.20	8
ATOM	2870	CD1	LEU	A	352	23.973	25.292	15.878	1.00	6.26	6	ATOM	2923	N	PRO	A	359	23.809	22.981	23.858	1.00	9.59	7
ATOM	2871	CD2	LEU	A	352	23.307	24.932	18.273	1.00	6.10	6	ATOM	2924	CD	PRO	A	359	22.503	22.784	23.206	1.00	9.74	6
ATOM	2872	C	LEU	A	352	21.377	21.209	17.097	1.00	7.69	6	ATOM	2925	CA	PRO	A	359	24.786	23.481	22.907	1.00	9.51	6
ATOM	2873	O	LEU	A	352	20.314	21.664	17.512	1.00	7.18	8	ATOM	2926	CB	PRO	A	359	24.249	23.201	21.495	1.00	9.51	6
ATOM	2874	N	THR	A	353	21.530	20.143	16.291	1.00	8.22	7	ATOM	2927	CG	PRO	A	359	22.763	23.211	21.778	1.00	9.71	6
ATOM	2875	CA	THR	A	353	20.394	19.372	15.781	1.00	9.02	6	ATOM	2928	C	PRO	A	359	25.173	24.945	23.045	1.00	9.55	6
ATOM	2876	CB	THR	A	353	20.420	19.145	14.234	1.00	9.08	6	ATOM	2929	O	PRO	A	359	24.319	25.756	23.334	1.00	9.40	8
ATOM	2877	OG1	THR	A	353	21.434	18.262	13.784	1.00	8.55	8	ATOM	2930	N	GLW	A	360	26.454	25.242	22.837	1.00	9.58	7
ATOM	2878	CG2	THR	A	353	20.559	20.504	13.545	1.00	9.72	6	ATOM	2931	CA	GLW	A	360	26.970	26.588	22.963	1.00	9.76	6
ATOM	2879	C	THR	A	353	20.161	18.030	16.481	1.00	9.71	6	ATOM	2932	CB	GLW	A	360	28.115	26.660	24.024	1.00	11.01	6
ATOM	2880	O	THR	A	353	19.066	17.453	16.250	1.00	9.88	8	ATOM	2933	CG	GLW	A	360	28.777	28.065	24.057	1.00	13.99	6
ATOM	2881	N	ARG	A	354	21.086	17.601	17.369	1.00	10.05	7	ATOM	2934	CD	GLW	A	360	30.282	28.033	24.332	1.00	15.99	6
ATOM	2882	CA	ARG	A	354	20.883	16.330	18.085	1.00	10.58	6	ATOM	2935	OE1	GLW	A	360	30.427	27.709	25.524	1.00	14.42	8
ATOM	2883	CB	ARG	A	354	22.258	15.688	18.208	1.00	9.90	6	ATOM	2936	NE2	GLW	A	360	31.291	28.336	23.425	1.00	15.78	7
ATOM	2884	CG	ARG	A	354	22.706	15.117	16.879	1.00	8.76	6	ATOM	2937	C	GLW	A	360	27.481	27.096	21.610	1.00	9.39	6
ATOM	2885	CD	ARG	A	354	24.107	14.517	17.011	1.00	9.60	6	ATOM	2938	O	GLW	A	360	28.228	26.305	21.007	1.00	9.32	8
ATOM	2886	CE	ARG	A	354	24.016	13.348	17.864	1.00	8.67	7	ATOM	2939	N	VAL	A	361	27.111	28.317	21.278	1.00	9.24	7
ATOM	2887	NZ	ARG	A	354	23.434	12.222	17.541	1.00	9.03	6	ATOM	2940	CA	VAL	A	361	27.586	28.925	20.022	1.00	9.26	6
ATOM	2888	NH1	ARG	A	354	23.392	11.309	18.513	1.00	10.30	7	ATOM	2941	CB	VAL	A	361	26.532	29.709	19.230	1.00	10.17	6
ATOM	2889	NH2	ARG	A	354	22.866	11.890	16.408	1.00	8.32	7	ATOM	2942	CG1	VAL	A	361	27.159	30.437	18.039	1.00	9.02	6
ATOM	2890	C	ARG	A	354	20.103	16.563	19.378	1.00	11.10	6	ATOM	2943	CG2	VAL	A	361	25.394	28.761	18.785	1.00	9.34	6
ATOM	2891	O	ARG	A	354	20.157	17.713	19.854	1.00	11.27	8	ATOM	2944	C	VAL	A	361	28.739	29.880	20.354	1.00	9.12	6
ATOM	2892	N	GLU	A	355	19.325	15.618	19.921	1.00	11.22	7	ATOM	2945	O	VAL	A	361	28.526	30.595	21.350	1.00	9.34	8
ATOM	2893	CA	GLU	A	355	18.560	15.818	21.130	1.00	11.61	6	ATOM	2946	N	PHE	A	362	30.879	29.887	19.703	1.00	8.60	7
ATOM	2894	CB	GLU	A	355	17.527	14.661	21.351	1.00	14.92	6	ATOM	2947	CA	PHE	A	362	32.308	30.768	20.056	1.00	8.23	6
ATOM	2895	CG	GLU	A	355	18.229	13.320	21.567	1.00	17.30	6	ATOM	2948	CB	PHE	A	362	32.308	30.060	19.804	1.00	5.00	6
ATOM	2896	CD	GLU	A	355	17.370	12.087	21.646	1.00	19.96	6	ATOM	2949	CG	PHE	A	362	33.606	30.771	20.058	1.00	6.40	6
ATOM	2897	OE1	GLU	A	355	17.828	10.936	21.901	1.00	21.87	8	ATOM	2950	CD1	PHE	A	362	33.778	31.642	21.142	1.00	5.78	6
ATOM	2898	OE2	GLU	A	355	16.145	12.138	21.394	1.00	22.12	8	ATOM	2951	CD2	PHE	A	362	34.710	30.563	19.197	1.00	5.00	6
ATOM	2899	C	GLU	A	355	19.317	15.898	22.469	1.00	11.55	6	ATOM	2952	CE1	PHE	A	362	34.961	32.330	21.423	1.00	5.15	6
ATOM	2900	O	GLU	A	355	18.718	16.405	23.441	1.00	11.55	8	ATOM	2953	CE2	PHE	A	362	35.912	31.220	19.464	1.00	5.23	6
ATOM	2901	N	SER	A	356	20.569	15.450	22.576	1.00	11.30	7	ATOM	2954	CZ	PHE	A	362	36.039	32.080	20.579	1.00	5.49	6
ATOM	2902	CA	SER	A	356	21.130	15.577	23.939	1.00	11.56	6	ATOM	2955	C	PHE	A	362	30.967	32.053	19.251	1.00	8.28	6
ATOM	2903	CG	SER	A	356	22.246	14.171	24.475	1.00	13.81	6	ATOM	2956	O	PHE	A	362	30.857	32.004	18.043	1.00	7.85	8
ATOM	2904	OG	SER	A	356	22.246	13.514	23.552	1.00	18.62	8	ATOM	2957	N	TYR	A	363	31.117	33.210	19.872	1.00	8.47	7
ATOM	2905	C	SER	A	356	22.241	16.607	23.975	1.00	11.33	6	ATOM	2958	CA	TYR	A	363	31.144	34.545	19.289	1.00	8.47	7
ATOM	2906	O	SER	A	356	22.863	16.940	22.971	1.00	11.70	8	ATOM	2959	CB	TYR	A	363	31.363	35.652	20.344	1.00	9.13	6
ATOM	2907	N	GLY	A	357	22.426	17.219	25.136	1.00	10.87	7	ATOM	2960	CG	TYR	A	363	31.530	37.091	19.976	1.00	9.86	6
ATOM	2908	CA	GLY	A	357	23.363	18.269	25.422	1.00	10.39	6	ATOM	2961	CD1	TYR	A	363	30.479	37.981	20.213	1.00	10.09	6
ATOM	2909	C	GLY	A	357	22.619	19.822	25.239	1.00	10.36	6	ATOM	2962	CE1	TYR	A	363	30.585	39.317	19.904	1.00	10.35	6
ATOM	2910	O	GLY	A	357	21.602	19.837	26.547	1.00	10.17	8	ATOM	2963	CD2	TYR	A	363	32.709	37.609	19.410	1.00	10.25	6
ATOM	2911	N	TYR	A	358	23.255	20.608	25.880	1.00	10.01	7	ATOM	2964	CE2	TYR	A	363	32.850	38.956	19.091	1.00	10.30	6
ATOM	2912	CA	TYR	A	358	22.884	22.017	25.877	1.00	9.76	6	ATOM	2965	CZ	TYR	A	363	31.776	39.774	19.365	1.00	10.78	6
ATOM	2913	CB	TYR	A	358	22.669	22.498	27.311	1.00	9.60	6	ATOM	2966	OH	TYR	A	363	31.831	41.126	19.087	1.00	11.58	8
ATOM	2914	CG	TYR	A	358	22.268	23.937	27.516	1.00	9.61	6	ATOM	2967	C	TYR	A	363	32.241	44.680	18.187	1.00	8.73	8
ATOM	2915	CD1	TYR	A	358	21.829	24.775	26.494	1.00	9.48	6	ATOM	2968	O	TYR	A	363	32.011	35.363	17.191	1.00	8.42	8

ATOM	2969	H	GLY A 364	33.399	34.040	18.452	1.00	8.56	7	ATOM	3022	CA	GLY A 371	43.889	37.991	16.742	1.00	22.15	6
ATOM	2970	CA	GLY A 364	34.472	34.061	17.503	1.00	8.81	6	ATOM	3023	C	GLY A 371	44.817	38.443	15.581	1.00	23.36	6
ATOM	2971	C	GLY A 364	34.083	33.251	16.231	1.00	9.04	6	ATOM	3024	O	GLY A 371	44.393	38.896	14.521	1.00	23.05	8
ATOM	2972	O	GLY A 364	34.596	33.639	15.156	1.00	8.91	8	ATOM	3025	N	ASP A 372	46.095	38.223	15.877	1.00	24.83	7
ATOM	2973	H	ASP A 365	31.233	32.251	16.327	1.00	9.21	7	ATOM	3026	CA	ASP A 372	47.186	38.626	15.016	1.00	26.55	6
ATOM	2974	CA	ASP A 365	32.830	31.513	15.137	1.00	9.93	6	ATOM	3027	CG	ASP A 372	48.323	39.306	15.968	1.00	31.39	6
ATOM	2975	C8	ASP A 365	32.255	30.146	15.429	1.00	8.93	6	ATOM	3028	CG	ASP A 372	47.962	40.791	15.968	1.00	31.39	6
ATOM	2976	CG	ASP A 365	33.369	29.235	15.977	1.00	9.58	6	ATOM	3029	CO1	ASP A 372	47.609	41.363	14.906	1.00	37.36	8
ATOM	2977	CO1	ASP A 365	34.516	29.422	15.641	1.00	10.56	8	ATOM	3030	CO2	ASP A 372	47.972	41.443	17.034	1.00	37.47	8
ATOM	2978	CO2	ASP A 365	33.078	28.275	16.700	1.00	9.75	8	ATOM	3031	C	ASP A 372	47.796	37.520	14.189	1.00	27.31	6
ATOM	2979	O	ASP A 365	31.780	32.264	16.321	1.00	10.69	6	ATOM	3032	O	ASP A 372	48.870	37.818	13.613	1.00	27.65	8
ATOM	2980	O	ASP A 365	31.770	32.135	13.078	1.00	10.75	8	ATOM	3033	H	SER A 373	47.162	36.353	14.146	1.00	27.64	7
ATOM	2981	H	MET A 366	30.887	32.996	14.980	1.00	11.30	7	ATOM	3034	CA	SER A 373	47.800	35.318	13.305	1.00	27.95	6
ATOM	2982	CA	MET A 366	29.857	33.792	14.295	1.00	11.93	6	ATOM	3035	C8	SER A 373	47.678	33.936	13.932	1.00	26.91	6
ATOM	2983	C8	MET A 366	28.838	34.351	15.303	1.00	14.14	6	ATOM	3036	CG	SER A 373	46.393	33.416	13.642	1.00	28.21	8
ATOM	2984	CG	MET A 366	27.828	33.348	15.827	1.00	17.97	6	ATOM	3037	C	SER A 373	47.255	35.373	11.873	1.00	28.20	6
ATOM	2985	SE	MET A 366	26.475	33.032	14.646	1.00	22.02	16	ATOM	3038	O	SER A 373	46.480	36.189	11.366	1.00	28.10	8
ATOM	2986	CE	MET A 366	25.576	34.590	14.752	1.00	20.61	6	ATOM	3039	N	GLN A 374	47.780	34.393	11.137	1.00	28.61	7
ATOM	2987	C	MET A 366	30.455	35.016	13.604	1.00	12.33	6	ATOM	3040	CA	GLN A 374	47.348	34.201	9.729	1.00	28.66	6
ATOM	2988	O	MET A 366	30.240	35.367	12.445	1.00	12.31	8	ATOM	3041	CG	GLN A 374	48.525	34.112	8.767	1.00	34.24	6
ATOM	2989	CA	TYR A 367	31.831	36.964	13.927	1.00	13.46	6	ATOM	3042	CG	GLN A 374	49.400	35.309	8.530	1.00	40.44	6
ATOM	2990	CA	TYR A 367	31.249	35.740	14.417	1.00	12.74	7	ATOM	3043	CD	GLN A 374	48.939	36.714	8.874	1.00	45.21	6
ATOM	2991	C	TYR A 367	31.548	38.085	14.988	1.00	14.31	6	ATOM	3044	OE1	GLN A 374	48.111	37.342	8.149	1.00	47.86	8
ATOM	2992	CG	TYR A 367	30.092	38.282	15.374	1.00	15.58	6	ATOM	3045	ME2	GLN A 374	49.449	37.277	10.005	1.00	45.97	7
ATOM	2993	CD1	TYR A 367	29.721	38.284	16.720	1.00	15.98	6	ATOM	3046	C	GLN A 374	46.414	32.963	9.719	1.00	28.21	6
ATOM	2994	CE1	TYR A 367	28.610	38.438	17.141	1.00	16.47	6	ATOM	3047	O	GLN A 374	46.105	32.340	8.674	1.00	28.76	8
ATOM	2995	CD2	TYR A 367	29.075	38.425	16.433	1.00	16.06	6	ATOM	3048	N	ARG A 375	45.952	32.517	10.873	1.00	26.96	7
ATOM	2996	CE2	TYR A 367	27.776	38.629	14.845	1.00	16.69	6	ATOM	3049	CA	ARG A 375	45.066	31.421	11.109	1.00	25.60	6
ATOM	2997	CZ	TYR A 367	27.431	38.644	16.196	1.00	16.89	6	ATOM	3050	CG	ARG A 375	45.641	30.394	12.115	1.00	29.84	6
ATOM	2998	OH	TYR A 367	26.105	38.815	16.553	1.00	16.92	8	ATOM	3051	C8	ARG A 375	46.842	29.713	11.509	1.00	33.73	6
ATOM	2999	O	TYR A 367	33.299	36.913	13.589	1.00	13.51	6	ATOM	3052	CD	ARG A 375	48.088	30.386	12.067	1.00	36.33	6
ATOM	3000	O	TYR A 367	33.233	38.005	13.190	1.00	13.49	8	ATOM	3053	WE	ARG A 375	48.286	30.141	13.475	1.00	37.64	7
ATOM	3001	H	GLY A 368	34.050	35.837	13.717	1.00	13.66	7	ATOM	3054	C2	ARG A 375	47.856	29.261	14.351	1.00	37.09	6
ATOM	3002	CA	GLY A 368	35.472	35.957	13.368	1.00	14.18	6	ATOM	3055	WH1	ARG A 375	47.016	28.308	13.998	1.00	37.77	7
ATOM	3003	C	GLY A 368	36.289	36.369	14.599	1.00	14.83	6	ATOM	3056	WH2	ARG A 375	48.293	29.399	15.587	1.00	36.83	7
ATOM	3004	O	GLY A 368	35.746	36.992	15.528	1.00	15.20	8	ATOM	3057	C	ARG A 375	43.777	31.845	11.827	1.00	23.88	6
ATOM	3005	N	THR A 369	37.531	35.971	14.691	1.00	14.98	7	ATOM	3058	O	ARG A 375	43.218	30.942	12.450	1.00	23.81	8
ATOM	3006	CA	THR A 369	38.409	36.330	15.759	1.00	15.75	6	ATOM	3059	N	GLU A 376	43.399	33.116	11.777	1.00	22.28	7
ATOM	3007	CB	THR A 369	39.185	35.126	16.318	1.00	14.06	6	ATOM	3060	CA	GLU A 376	42.196	33.558	12.450	1.00	20.37	6
ATOM	3008	OG1	THR A 369	39.926	34.392	15.324	1.00	11.76	8	ATOM	3061	CB	GLU A 376	42.061	35.080	12.418	1.00	17.56	6
ATOM	3009	CG2	THR A 369	38.175	34.186	16.966	1.00	10.90	6	ATOM	3062	CG	GLU A 376	43.203	35.780	13.151	1.00	16.13	6
ATOM	3010	C	THR A 369	39.346	37.437	15.225	1.00	16.84	6	ATOM	3063	CG	GLU A 376	43.361	35.421	14.595	1.00	14.90	6
ATOM	3011	O	THR A 369	39.727	37.463	16.039	1.00	16.53	8	ATOM	3064	OE1	GLU A 376	42.403	35.436	15.391	1.00	12.95	8
ATOM	3012	N	LYS A 370	39.733	38.369	16.120	1.00	17.86	7	ATOM	3065	OE2	GLU A 376	44.510	35.108	15.051	1.00	16.10	8
ATOM	3013	CA	LYS A 370	40.568	39.488	15.712	1.00	19.14	6	ATOM	3066	C	GLU A 376	40.955	32.886	11.869	1.00	19.17	6
ATOM	3014	CB	LYS A 370	39.849	40.792	16.133	1.00	22.20	6	ATOM	3067	O	GLU A 376	40.801	32.503	10.715	1.00	18.94	8
ATOM	3015	CG	LYS A 370	38.702	41.073	15.133	1.00	26.42	6	ATOM	3068	N	ILE A 377	40.002	32.698	12.777	1.00	18.23	7
ATOM	3016	CD	LYS A 370	39.254	41.271	13.736	1.00	29.66	6	ATOM	3069	CA	ILE A 377	38.726	32.102	12.410	1.00	17.23	6
ATOM	3017	CE	LYS A 370	38.326	41.239	12.544	1.00	32.10	7	ATOM	3070	CG2	ILE A 377	37.924	31.634	13.636	1.00	15.28	6
ATOM	3018	HZ	LYS A 370	39.111	41.178	11.243	1.00	33.93	7	ATOM	3071	CG1	ILE A 377	36.616	30.961	13.205	1.00	15.23	6
ATOM	3019	C	LYS A 370	41.998	39.442	16.214	1.00	19.90	6	ATOM	3072	CG1	ILE A 377	38.720	30.715	14.564	1.00	14.23	6
ATOM	3020	O	LYS A 370	42.638	40.436	16.526	1.00	19.78	8	ATOM	3073	CD1	ILE A 377	38.109	30.512	15.935	1.00	13.53	6
ATOM	3021	N	GLY A 371	42.534	38.244	16.329	1.00	20.85	7	ATOM	3074	C	ILE A 377	37.957	33.184	11.660	1.00	16.78	6

SUBSTITUTE SHEET (RULE 26)

ATOM	3075	O	ILE A 377	37.783	34.301	12.173	1.00	16.90	6
ATOM	3076	H	PRO A 378	37.461	32.927	10.461	1.00	16.21	7
ATOM	3077	CD	PRO A 378	37.634	31.617	9.821	1.00	16.04	6
ATOM	3078	CA	PRO A 378	36.637	33.810	9.695	1.00	15.87	6
ATOM	3079	CB	PRO A 378	36.555	33.232	8.263	1.00	15.98	6
ATOM	3080	CG	PRO A 378	37.023	31.835	8.456	1.00	15.94	6
ATOM	3081	C	PRO A 378	35.214	33.860	10.247	1.00	15.56	6
ATOM	3082	O	PRO A 378	34.741	32.945	10.946	1.00	15.55	8
ATOM	3083	H	ALA A 379	34.506	34.960	9.931	1.00	15.19	7
ATOM	3084	CA	ALA A 379	33.095	35.063	10.370	1.00	14.83	6
ATOM	3085	CB	ALA A 379	32.523	36.450	10.119	1.00	13.37	6
ATOM	3086	C	ALA A 379	32.246	33.979	9.679	1.00	14.60	6
ATOM	3087	O	ALA A 379	32.082	33.990	8.438	1.00	14.28	7
ATOM	3088	H	LEU A 380	31.703	33.021	10.428	1.00	14.28	6
ATOM	3089	CA	LEU A 380	30.925	31.960	9.792	1.00	14.14	6
ATOM	3090	CG	LEU A 380	31.468	30.617	10.265	1.00	15.00	6
ATOM	3091	CD	LEU A 380	32.913	30.303	9.865	1.00	16.56	6
ATOM	3092	CD1	LEU A 380	33.486	29.165	10.668	1.00	16.26	6
ATOM	3093	CD2	LEU A 380	32.975	30.004	8.350	1.00	16.68	6
ATOM	3094	C	LEU A 380	29.448	32.123	10.017	1.00	14.34	6
ATOM	3095	O	LEU A 380	28.602	31.262	9.773	1.00	14.38	8
ATOM	3096	H	LYS A 381	29.011	33.278	10.475	1.00	14.36	7
ATOM	3097	CA	LYS A 381	27.615	33.579	10.719	1.00	14.84	6
ATOM	3098	CB	LYS A 381	27.672	35.101	10.820	1.00	18.02	6
ATOM	3099	CG	LYS A 381	26.382	35.855	10.702	1.00	21.47	6
ATOM	3100	CD	LYS A 381	26.754	37.314	10.944	1.00	25.20	6
ATOM	3101	C	LYS A 381	25.912	38.275	10.770	1.00	20.81	6
ATOM	3102	H2	LYS A 381	24.564	38.411	10.770	1.00	30.73	7
ATOM	3103	C	LYS A 381	26.667	33.106	9.634	1.00	14.98	6
ATOM	3104	O	LYS A 381	25.589	32.577	9.911	1.00	14.84	8
ATOM	3105	H	HIS A 382	26.978	33.273	8.350	1.00	14.98	7
ATOM	3106	CA	HIS A 382	26.079	32.889	7.268	1.00	15.22	6
ATOM	3107	CB	HIS A 382	26.562	33.593	5.986	1.00	21.24	6
ATOM	3108	CG	HIS A 382	28.036	33.424	5.842	1.00	25.72	6
ATOM	3109	CD	HIS A 382	29.070	32.878	6.615	1.00	27.36	6
ATOM	3110	WD1	HIS A 382	28.569	32.671	6.810	1.00	28.03	7
ATOM	3111	CE1	HIS A 382	29.903	32.712	4.939	1.00	28.96	6
ATOM	3112	ME2	HIS A 382	30.216	33.424	6.061	1.00	28.60	7
ATOM	3113	C	HIS A 382	25.947	31.415	7.118	1.00	15.05	6
ATOM	3114	O	HIS A 382	24.948	30.932	6.602	1.00	15.08	8
ATOM	3115	H	LYS A 383	26.887	30.595	7.622	1.00	14.36	6
ATOM	3116	CA	LYS A 383	26.802	29.161	7.615	1.00	14.36	6
ATOM	3117	CB	LYS A 383	28.186	28.551	7.528	1.00	16.14	6
ATOM	3118	CG	LYS A 383	29.014	29.281	6.505	1.00	20.51	6
ATOM	3119	CD	LYS A 383	29.147	28.507	5.230	1.00	23.48	6
ATOM	3120	CE	LYS A 383	30.673	28.350	4.977	1.00	26.30	6
ATOM	3121	H2	LYS A 383	31.046	29.207	3.792	1.00	27.91	7
ATOM	3122	O	LYS A 383	26.207	28.595	8.926	1.00	13.88	6
ATOM	3123	C	LYS A 383	25.694	27.478	8.956	1.00	13.80	8
ATOM	3124	H	ILE A 384	26.351	29.374	10.004	1.00	13.23	7
ATOM	3125	CA	ILE A 384	25.814	28.889	11.252	1.00	12.99	6
ATOM	3126	CB	ILE A 384	26.609	29.381	12.486	1.00	13.25	6
ATOM	3127	CG2	ILE A 384	25.905	29.000	13.778	1.00	12.19	6
ATOM	3128	CG1	ILE A 384	28.029	28.790	12.411	1.00	13.70	6
ATOM	3129	CD1	ILE A 384	28.902	29.649	13.343	1.00	15.12	6
ATOM	3130	C	ILE A 384	24.355	29.241	11.430	1.00	12.61	6
ATOM	3131	O	ILE A 384	23.621	28.363	11.931	1.00	12.68	8
ATOM	3132	N	GLU A 385	23.841	30.401	11.025	1.00	12.22	7
ATOM	3133	CA	GLU A 385	22.459	30.804	11.178	1.00	12.09	6
ATOM	3134	CB	GLU A 385	22.249	32.252	10.671	1.00	13.25	6
ATOM	3135	CG	GLU A 385	23.039	33.148	11.637	1.00	16.06	6
ATOM	3136	CD	GLU A 385	22.681	34.621	11.531	1.00	18.04	6
ATOM	3137	OE1	GLU A 385	22.082	35.050	10.531	1.00	18.27	8
ATOM	3138	OE2	GLU A 385	22.960	35.427	12.453	1.00	18.60	8
ATOM	3139	C	GLU A 385	21.439	29.867	10.587	1.00	11.96	6
ATOM	3140	O	GLU A 385	20.439	29.608	11.273	1.00	12.04	8
ATOM	3141	N	PRO A 386	21.614	29.238	9.436	1.00	11.74	7
ATOM	3142	CD	PRO A 386	22.735	29.467	8.528	1.00	11.74	6
ATOM	3143	CA	PRO A 386	20.676	28.265	8.905	1.00	11.52	6
ATOM	3144	CB	PRO A 386	21.205	27.847	7.516	1.00	11.54	6
ATOM	3145	CG	PRO A 386	22.167	28.967	7.199	1.00	11.74	6
ATOM	3146	C	PRO A 386	20.545	27.050	9.826	1.00	11.28	6
ATOM	3147	O	PRO A 386	19.493	26.419	9.963	1.00	11.21	8
ATOM	3148	N	ILE A 387	21.617	26.648	10.530	1.00	11.05	7
ATOM	3149	CA	ILE A 387	21.619	25.492	11.424	1.00	10.84	6
ATOM	3150	CB	ILE A 387	23.047	24.957	11.653	1.00	8.79	6
ATOM	3151	CG1	ILE A 387	22.978	23.619	12.340	1.00	6.90	6
ATOM	3152	CG2	ILE A 387	23.799	24.850	10.310	1.00	8.27	6
ATOM	3153	CD1	ILE A 387	25.231	24.430	10.511	1.00	9.38	6
ATOM	3154	C	ILE A 387	20.917	25.808	12.754	1.00	11.01	6
ATOM	3155	O	ILE A 387	20.273	24.946	13.366	1.00	10.92	8
ATOM	3156	N	LEU A 388	21.058	27.064	13.176	1.00	11.09	7
ATOM	3157	CA	LEU A 388	20.400	27.620	14.345	1.00	11.19	6
ATOM	3158	CB	LEU A 388	20.902	29.010	14.682	1.00	10.46	6
ATOM	3159	CG	LEU A 388	22.084	29.061	15.638	1.00	11.84	6
ATOM	3160	CD1	LEU A 388	22.502	30.545	15.745	1.00	11.69	6
ATOM	3161	CD2	LEU A 388	21.636	28.377	16.916	1.00	10.70	6
ATOM	3162	C	LEU A 388	18.887	27.688	14.042	1.00	11.21	6
ATOM	3163	O	LYS A 389	18.017	27.443	14.899	1.00	11.36	6
ATOM	3164	N	LYS A 389	18.551	28.015	12.792	1.00	11.22	7
ATOM	3165	CA	LYS A 389	17.142	28.017	12.353	1.00	11.08	6
ATOM	3166	CB	LYS A 389	17.014	28.553	10.952	1.00	14.65	6
ATOM	3167	CG	LYS A 389	15.591	28.665	10.402	1.00	20.09	6
ATOM	3168	CD	LYS A 389	15.454	30.134	9.985	1.00	24.33	6
ATOM	3169	CE	LYS A 389	14.860	30.232	8.592	1.00	27.30	6
ATOM	3170	N2	LYS A 389	13.649	29.337	8.568	1.00	30.42	7
ATOM	3171	O	LYS A 389	16.620	26.566	12.377	1.00	10.52	6
ATOM	3172	C	LYS A 389	15.474	26.300	12.746	1.00	10.45	8
ATOM	3173	N	ALA A 390	17.445	25.613	11.937	1.00	10.03	7
ATOM	3174	CA	ALA A 390	17.007	24.226	12.020	1.00	9.88	6
ATOM	3175	CB	ALA A 390	17.970	23.263	11.375	1.00	7.86	6
ATOM	3176	C	ALA A 390	16.848	23.832	13.506	1.00	9.86	6
ATOM	3177	O	ALA A 390	15.876	23.103	13.761	1.00	9.92	8
ATOM	3178	N	ARG A 391	17.713	24.258	14.440	1.00	9.66	7
ATOM	3179	CA	ARG A 391	17.540	23.914	15.857	1.00	9.64	6
ATOM	3180	CB	ARG A 391	18.666	24.410	16.800	1.00	8.27	6

SUBSTITUTE SHEET (RULE 26)

ATOM	3181	CG	ARG A 391	18.295	24.255	18.295	1.00	6.17	6
ATOM	3182	CD	ARG A 391	19.637	24.301	19.079	1.00	6.11	6
ATOM	3183	NE	ARG A 391	19.415	23.982	20.476	1.00	6.39	7
ATOM	3184	CZ	ARG A 391	19.411	22.752	21.057	1.00	8.41	6
ATOM	3185	HH1	ARG A 391	19.671	21.719	20.264	1.00	7.01	7
ATOM	3186	HH2	ARG A 391	19.147	22.533	22.359	1.00	6.75	7
ATOM	3187	C	ARG A 391	16.258	24.518	16.434	1.00	9.84	6
ATOM	3188	O	ARG A 391	15.482	23.660	17.089	1.00	9.35	8
ATOM	3189	N	LYS A 392	16.061	25.811	16.184	1.00	10.42	7
ATOM	3190	CA	LYS A 392	14.904	26.555	16.666	1.00	11.31	6
ATOM	3191	CB	LYS A 392	15.137	28.036	16.253	1.00	13.27	6
ATOM	3192	CG	LYS A 392	14.066	28.928	16.797	1.00	16.07	6
ATOM	3193	CD	LYS A 392	14.176	30.388	16.369	1.00	20.09	6
ATOM	3194	CE	LYS A 392	12.989	31.069	16.665	1.00	23.10	6
ATOM	3195	NZ	LYS A 392	13.536	32.560	16.682	1.00	26.05	7
ATOM	3196	C	LYS A 392	12.091	25.218	14.386	1.00	11.94	6
ATOM	3197	O	LYS A 392	13.349	25.676	14.916	1.00	11.92	8
ATOM	3198	N	GLN A 393	12.091	25.218	14.386	1.00	12.80	6
ATOM	3199	CA	GLN A 393	11.736	25.947	13.069	1.00	17.13	6
ATOM	3200	CB	GLN A 393	12.463	27.237	12.917	1.00	26.67	6
ATOM	3201	CG	GLN A 393	11.701	28.402	12.316	1.00	29.33	6
ATOM	3202	CD	GLN A 393	11.924	28.717	11.149	1.00	30.64	8
ATOM	3203	DE1	GLN A 393	10.856	29.003	13.159	1.00	31.70	7
ATOM	3204	DE2	GLN A 393	11.921	23.744	13.940	1.00	12.57	6
ATOM	3205	C	GLN A 393	12.995	23.041	13.678	1.00	11.99	7
ATOM	3206	O	GLN A 394	12.839	21.690	13.167	1.00	11.56	6
ATOM	3207	N	TYR A 394	13.577	21.661	11.798	1.00	11.71	6
ATOM	3208	CA	TYR A 394	12.942	22.687	10.852	1.00	12.27	6
ATOM	3210	CG	TYR A 394	13.444	23.941	10.588	1.00	12.30	6
ATOM	3211	CE1	TYR A 394	12.811	24.826	9.747	1.00	12.61	6
ATOM	3212	CE2	TYR A 394	11.754	22.328	10.236	1.00	12.73	6
ATOM	3213	CD2	TYR A 394	11.066	23.192	9.378	1.00	13.02	6
ATOM	3215	CZ	TYR A 394	11.615	24.442	9.136	1.00	13.05	6
ATOM	3216	OH	TYR A 394	10.942	25.224	8.229	1.00	13.25	8
ATOM	3217	C	TYR A 394	13.360	20.552	14.017	1.00	11.27	6
ATOM	3218	O	TYR A 394	12.866	19.424	13.834	1.00	10.94	8
ATOM	3219	N	ALA A 395	14.338	20.794	14.908	1.00	10.88	7
ATOM	3220	CA	ALA A 395	16.305	20.151	16.074	1.00	10.74	6
ATOM	3221	CB	ALA A 395	14.101	19.267	16.920	1.00	10.85	6
ATOM	3222	C	ALA A 395	12.986	18.545	16.743	1.00	10.85	7
ATOM	3223	O	ALA A 395	12.061	18.070	17.753	1.00	10.83	6
ATOM	3225	CA	TYR A 396	10.763	18.949	17.821	1.00	10.80	6
ATOM	3226	CB	TYR A 396	11.083	20.390	18.180	1.00	10.52	6
ATOM	3227	CG	TYR A 396	11.333	21.365	17.195	1.00	10.49	6
ATOM	3228	CD1	TYR A 396	11.683	22.665	17.546	1.00	10.24	6
ATOM	3229	CE1	TYR A 396	11.215	20.744	19.504	1.00	10.26	6
ATOM	3230	CD2	TYR A 396	11.536	22.043	19.835	1.00	10.18	6
ATOM	3231	CE2	TYR A 396	11.799	22.984	18.874	1.00	10.23	6
ATOM	3232	CZ	TYR A 396	12.200	24.237	19.305	1.00	10.59	8
ATOM	3233	OH	TYR A 396						
ATOM	3234	C	TYR A 396	11.624	16.631	17.499	1.00	10.90	6
ATOM	3235	O	TYR A 396	11.615	16.137	16.372	1.00	10.58	8
ATOM	3236	N	GLY A 397	11.252	15.899	18.555	1.00	11.07	7
ATOM	3237	CA	GLY A 397	10.772	14.542	18.296	1.00	11.32	6
ATOM	3238	C	GLY A 397	11.808	13.450	18.353	1.00	11.58	6
ATOM	3239	O	GLY A 397	13.001	13.761	18.466	1.00	12.00	8
ATOM	3240	N	ALA A 398	11.341	12.228	18.304	1.00	11.57	7
ATOM	3241	CA	ALA A 398	12.172	11.044	18.341	1.00	11.80	6
ATOM	3242	CB	ALA A 398	11.261	9.824	18.105	1.00	9.85	6
ATOM	3243	C	ALA A 398	13.348	11.115	17.365	1.00	12.04	6
ATOM	3244	O	ALA A 398	13.259	11.447	16.176	1.00	12.09	8
ATOM	3245	N	GLM A 399	14.532	10.718	17.833	1.00	12.00	7
ATOM	3246	CA	GLM A 399	15.761	10.691	17.058	1.00	12.04	6
ATOM	3247	CB	GLM A 399	16.871	11.357	17.912	1.00	10.48	6
ATOM	3248	CG	GLM A 399	18.261	11.287	17.346	1.00	9.54	6
ATOM	3249	CD	GLM A 399	19.195	12.269	18.066	1.00	9.97	6
ATOM	3250	DE1	GLM A 399	18.983	13.467	18.191	1.00	8.29	8
ATOM	3251	DE2	GLM A 399	20.306	11.751	18.528	1.00	9.30	7
ATOM	3252	C	GLM A 399	16.212	9.307	16.643	1.00	12.27	6
ATOM	3253	O	GLM A 399	16.138	8.327	17.361	1.00	12.29	8
ATOM	3254	N	HIS A 400	17.765	9.135	15.415	1.00	12.36	7
ATOM	3255	CA	HIS A 400	17.270	7.893	14.903	1.00	12.28	6
ATOM	3256	CB	HIS A 400	16.419	7.243	13.800	1.00	12.34	6
ATOM	3257	CG	HIS A 400	15.001	6.998	14.252	1.00	13.76	6
ATOM	3258	CD2	HIS A 400	14.464	6.087	15.135	1.00	12.53	6
ATOM	3259	HD1	HIS A 400	13.959	7.856	13.831	1.00	13.34	7
ATOM	3260	CE1	HIS A 400	12.860	7.408	14.435	1.00	11.97	6
ATOM	3261	ME2	HIS A 400	13.095	6.378	15.194	1.00	11.69	7
ATOM	3262	C	HIS A 400	18.710	8.179	14.411	1.00	12.21	6
ATOM	3263	O	HIS A 400	18.909	9.132	13.670	1.00	11.78	8
ATOM	3264	N	ASP A 401	19.651	7.332	14.895	1.00	12.31	7
ATOM	3265	CA	ASP A 401	21.043	7.503	14.536	1.00	15.32	6
ATOM	3266	CB	ASP A 401	21.683	8.427	16.767	1.00	18.10	6
ATOM	3268	CD1	ASP A 401	21.438	9.578	16.520	1.00	20.24	8
ATOM	3269	CD2	ASP A 401	22.299	8.187	17.921	1.00	19.29	8
ATOM	3270	C	ASP A 401	21.556	6.515	13.484	1.00	12.57	6
ATOM	3271	O	ASP A 401	21.145	5.360	13.483	1.00	12.31	8
ATOM	3272	N	TYR A 402	22.385	6.972	12.584	1.00	12.55	7
ATOM	3273	CA	TYR A 402	22.977	6.173	11.524	1.00	12.83	6
ATOM	3274	CB	TYR A 402	22.385	6.495	10.130	1.00	12.68	6
ATOM	3275	CG	TYR A 402	20.891	6.179	10.105	1.00	12.98	6
ATOM	3276	CD	TYR A 402	19.990	7.186	10.470	1.00	13.23	6
ATOM	3277	CE1	TYR A 402	18.631	6.952	10.544	1.00	13.64	6
ATOM	3278	CE2	TYR A 402	20.378	4.927	9.801	1.00	13.10	6
ATOM	3279	OH	TYR A 402	19.018	4.654	9.819	1.00	13.39	6
ATOM	3280	C	TYR A 402	18.168	5.676	10.195	1.00	14.02	6
ATOM	3281	CA	TYR A 402	16.795	5.502	10.282	1.00	14.72	8
ATOM	3282	CB	TYR A 402	24.476	6.371	11.592	1.00	13.30	6
ATOM	3283	O	TYR A 402	25.019	7.054	10.747	1.00	13.17	8
ATOM	3284	N	PHE A 403	25.162	5.818	12.581	1.00	14.08	7
ATOM	3285	CA	PHE A 403	26.591	5.861	12.792	1.00	14.73	6
ATOM	3286	CB	PHE A 403	26.978	6.035	14.266	1.00	16.26	6

ATOM	3287	CG	PHE A 403	7.486	14.665	1.00	19.71	6	26.766	9.309	9.436	27.012	9.309	1.00	11.68	6
ATOM	3288	CD1	PHE A 403	7.927	15.176	1.00	20.07	6	25.574	10.638	9.616	27.735	10.638	1.00	13.02	6
ATOM	3289	CD2	PHE A 403	8.440	14.483	1.00	21.01	6	27.748	10.804	8.661	28.916	10.804	1.00	14.14	6
ATOM	3290	CD1	PHE A 403	25.379	15.534	1.00	21.01	6	25.379	10.817	11.030	28.293	10.817	1.00	11.59	6
ATOM	3291	CD2	PHE A 403	27.540	9.786	1.00	22.26	6	27.540	10.380	10.380	25.823	10.380	1.00	11.38	6
ATOM	3292	CZ	PHE A 403	26.338	10.216	1.00	21.47	6	26.338	11.441	8.613	25.887	11.441	1.00	11.38	8
ATOM	3293	C	PHE A 403	27.113	4.537	1.00	15.16	6	27.113	10.000	9.898	24.747	10.000	1.00	10.96	7
ATOM	3294	O	PHE A 403	27.616	3.625	1.00	15.23	8	27.616	10.842	9.910	23.548	10.842	1.00	10.41	6
ATOM	3295	H	ASP A 404	26.987	4.370	1.00	15.33	7	26.987	10.508	11.084	22.635	10.508	1.00	9.89	6
ATOM	3296	CA	ASP A 404	27.398	3.103	1.00	15.59	6	27.398	11.830	9.547	22.871	11.830	1.00	9.60	8
ATOM	3297	CB	ASP A 404	26.115	2.428	1.00	17.33	6	26.115	11.347	11.201	21.623	11.347	1.00	9.60	7
ATOM	3298	CG	ASP A 404	25.433	3.431	1.00	19.38	6	25.433	11.201	12.204	20.569	11.201	1.00	9.34	6
ATOM	3299	CD1	ASP A 404	25.870	4.570	1.00	19.96	8	25.870	11.750	13.574	20.994	11.750	1.00	8.12	6
ATOM	3300	CD2	ASP A 404	28.346	3.116	1.00	15.47	6	28.346	13.662	13.285	22.726	13.662	1.00	8.48	6
ATOM	3301	C	ASP A 404	28.339	2.154	1.00	15.71	8	28.339	15.049	13.356	22.699	15.049	1.00	8.47	6
ATOM	3302	O	ASP A 404	30.098	4.238	1.00	14.80	6	30.098	13.010	12.971	23.924	13.010	1.00	9.18	6
ATOM	3303	CA	HIS A 405	29.168	8.997	1.00	15.11	7	29.168	14.285	13.808	20.647	14.285	1.00	6.27	6
ATOM	3304	CB	HIS A 405	29.332	4.915	1.00	14.80	6	29.332	15.439	13.671	21.483	15.439	1.00	6.58	7
ATOM	3305	CG	HIS A 405	30.187	4.926	1.00	15.21	6	30.187	13.113	12.732	25.054	13.814	1.00	9.15	6
ATOM	3306	CD1	HIS A 405	30.385	3.954	1.00	15.68	6	30.385	15.839	13.113	23.830	15.839	1.00	9.35	6
ATOM	3307	CD2	HIS A 405	30.992	5.990	1.00	15.84	7	30.992	15.163	12.799	25.007	15.163	1.00	9.69	6
ATOM	3308	HD1	HIS A 405	31.654	5.723	1.00	15.84	7	31.654	11.897	11.708	19.296	11.897	1.00	9.23	6
ATOM	3309	CE1	HIS A 405	31.309	4.491	1.00	17.15	7	31.309	12.824	10.901	19.372	12.824	1.00	8.76	9
ATOM	3310	NE2	HIS A 405	31.280	5.023	1.00	14.46	6	31.280	11.418	12.226	18.151	11.418	1.00	9.36	7
ATOM	3311	C	HIS A 405	31.008	5.908	1.00	14.63	8	31.008	12.015	11.894	16.877	12.015	1.00	9.69	6
ATOM	3312	H	HIS A 406	32.494	7.963	1.00	14.11	7	32.494	11.081	11.040	15.968	11.081	1.00	10.82	6
ATOM	3313	CA	HIS A 406	33.630	5.587	1.00	13.78	6	33.630	9.914	11.826	15.687	9.914	1.00	12.10	8
ATOM	3314	CB	HIS A 406	35.000	4.932	1.00	15.67	6	35.000	10.613	9.743	16.614	10.613	1.00	9.28	6
ATOM	3315	CG	HIS A 406	34.981	4.416	1.00	16.76	6	34.981	12.441	13.173	16.136	12.441	1.00	9.93	6
ATOM	3316	CD1	HIS A 406	34.450	3.285	1.00	16.51	6	34.450	12.027	14.318	16.399	12.027	1.00	9.78	8
ATOM	3317	CD2	HIS A 406	35.504	5.164	1.00	18.12	7	35.504	14.332	14.035	15.184	13.843	1.00	10.76	6
ATOM	3318	HD1	HIS A 406	35.318	4.505	1.00	16.95	6	35.318	14.635	14.615	14.635	14.635	1.00	8.23	6
ATOM	3319	ME2	HIS A 406	33.580	7.002	1.00	13.47	6	33.580	15.382	15.182	16.039	15.382	1.00	6.55	6
ATOM	3320	C	HIS A 406	34.298	7.753	1.00	13.10	8	34.298	16.262	14.604	16.262	14.604	1.00	6.58	6
ATOM	3321	O	HIS A 406	32.637	7.500	1.00	13.42	7	32.637	15.388	14.982	15.388	14.982	1.00	5.58	7
ATOM	3322	CA	ASP A 407	33.163	9.063	1.00	14.59	6	33.163	15.602	18.326	14.602	16.370	1.00	7.49	7
ATOM	3323	CB	ASP A 407	33.474	8.665	1.00	16.23	8	33.474	16.645	16.870	16.645	16.870	1.00	7.65	7
ATOM	3324	CG	ASP A 407	34.808	8.466	1.00	18.38	8	34.808	12.946	13.767	12.946	13.767	1.00	11.41	6
ATOM	3325	CD1	ASP A 407	31.457	9.532	1.00	12.98	6	31.457	14.374	12.355	12.678	14.374	1.00	11.24	8
ATOM	3326	CD2	ASP A 407	31.310	7.360	1.00	12.77	8	31.310	12.076	14.035	12.076	12.980	1.00	12.08	7
ATOM	3327	C	ASP A 407	30.645	8.890	1.00	12.85	7	30.645	10.713	13.510	9.957	11.626	1.00	12.84	6
ATOM	3328	CA	ASP A 407	29.098	9.438	1.00	12.79	6	29.098	10.578	13.880	10.578	10.270	1.00	11.98	6
ATOM	3329	CB	ASP A 407	28.429	9.103	1.00	14.07	6	28.429	9.722	14.401	9.722	14.401	1.00	12.67	6
ATOM	3330	CG	ASP A 407	27.045	9.742	1.00	13.86	6	27.045	8.485	14.504	8.485	9.240	1.00	14.73	8
ATOM	3331	CD1	ASP A 407	29.251	3.597	1.00	13.69	6	29.251	10.240	16.723	10.240	8.041	1.00	15.78	8
ATOM	3332	CD2	ASP A 407	28.979	8.781	1.00	14.63	6	28.979	9.819	13.605	9.819	14.015	1.00	13.32	8
ATOM	3333	C	ASP A 407	28.219	8.885	1.00	12.60	6	28.219	8.855	14.006	8.855	14.006	1.00	13.17	8
ATOM	3334	O	ASP A 407	27.838	7.712	1.00	12.81	8	27.838	10.096	16.389	10.096	15.006	1.00	14.06	7
ATOM	3335	H	VAL A 409	27.910	8.762	1.00	12.05	7	27.910	16.150	14.467	9.223	16.150	1.00	15.71	6

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ATOM	3393	C	GLY A 415	8.276	15.870	15.637	1.00	17.18	6
ATOM	3394	O	GLY A 415	8.176	14.768	16.148	1.00	17.23	8
ATOM	3395	N	ASP A 416	7.581	16.904	16.048	1.00	18.70	7
ATOM	3396	CA	ASP A 416	6.606	16.860	17.118	1.00	20.18	6
ATOM	3397	CB	ASP A 416	7.228	17.531	18.307	1.00	20.18	6
ATOM	3398	CG	ASP A 416	6.358	17.615	19.535	1.00	31.33	6
ATOM	3399	CD	ASP A 416	6.791	18.402	20.613	1.00	35.28	6
ATOM	3400	DD	ASP A 416	5.301	16.975	19.696	1.00	32.88	8
ATOM	3401	O	ASP A 416	5.400	17.597	16.568	1.00	21.08	6
ATOM	3402	N	SER A 417	5.423	18.631	15.908	1.00	21.08	6
ATOM	3403	CA	SER A 417	4.234	17.031	16.824	1.00	23.16	7
ATOM	3404	CB	SER A 417	2.928	17.484	16.380	1.00	23.16	6
ATOM	3405	CG	SER A 417	1.868	16.471	16.846	1.00	27.52	6
ATOM	3406	OG	SER A 417	1.734	16.874	18.237	1.00	32.78	8
ATOM	3407	C	SER A 417	2.585	18.852	16.929	1.00	23.50	6
ATOM	3408	O	SER A 417	1.821	19.541	16.258	1.00	23.90	8
ATOM	3409	N	SER A 418	3.145	19.217	18.073	1.00	23.61	7
ATOM	3410	CA	SER A 418	2.982	20.541	18.628	1.00	23.56	6
ATOM	3411	CB	SER A 418	3.267	20.523	20.135	1.00	24.90	6
ATOM	3412	CG	SER A 418	4.660	20.195	20.198	1.00	27.24	8
ATOM	3413	C	SER A 418	3.988	21.525	18.023	1.00	23.37	6
ATOM	3414	O	SER A 418	3.995	22.714	18.503	1.00	23.96	8
ATOM	3415	N	VAL A 419	4.894	21.195	17.094	1.00	22.44	7
ATOM	3416	CA	VAL A 419	5.793	22.233	16.490	1.00	21.33	6
ATOM	3417	CB	VAL A 419	7.278	22.269	16.815	1.00	19.53	6
ATOM	3418	CG	VAL A 419	8.070	23.317	16.038	1.00	15.95	6
ATOM	3419	CD	VAL A 419	7.558	22.527	18.315	1.00	18.97	6
ATOM	3420	C	VAL A 419	5.477	21.951	14.988	1.00	20.67	6
ATOM	3421	O	VAL A 419	5.911	20.939	14.404	1.00	20.45	8
ATOM	3422	N	ALA A 420	4.616	22.803	14.400	1.00	20.01	7
ATOM	3423	CA	ALA A 420	4.174	22.558	13.017	1.00	19.28	6
ATOM	3424	CB	ALA A 420	3.189	23.619	12.527	1.00	19.92	6
ATOM	3425	C	ALA A 420	5.329	22.464	12.050	1.00	18.43	6
ATOM	3426	O	ALA A 420	6.221	23.297	12.166	1.00	18.43	8
ATOM	3427	N	ASN A 421	5.312	21.471	11.161	1.00	17.67	7
ATOM	3428	CA	ASN A 421	6.356	21.242	10.168	1.00	16.69	6
ATOM	3429	CB	ASN A 421	6.537	22.436	9.204	1.00	19.20	6
ATOM	3430	CG	ASN A 421	5.312	22.617	8.330	1.00	21.29	6
ATOM	3431	CD	ASN A 421	4.586	21.711	7.966	1.00	22.05	8
ATOM	3432	C	ASN A 421	5.028	23.853	7.994	1.00	23.75	7
ATOM	3433	O	ASN A 421	7.760	20.891	10.703	1.00	15.64	6
ATOM	3434	N	SER A 422	8.711	20.946	9.931	1.00	15.23	8
ATOM	3435	CA	SER A 422	7.882	20.479	11.947	1.00	14.78	7
ATOM	3436	CB	SER A 422	9.140	20.088	12.542	1.00	14.31	6
ATOM	3437	CG	SER A 422	7.990	19.345	14.623	1.00	13.80	6
ATOM	3438	OG	SER A 422	7.990	18.705	12.009	1.00	13.67	8
ATOM	3439	C	SER A 422	8.713	17.932	11.459	1.00	13.79	6
ATOM	3440	O	SER A 422	10.797	18.389	12.161	1.00	12.94	7
ATOM	3441	N	GLY A 423	11.329	17.086	11.679	1.00	12.05	6
ATOM	3442	CA	GLY A 423	12.546	17.472	10.825	1.00	11.56	6
ATOM	3443	C	GLY A 423	12.532	18.566	10.232	1.00	11.46	8
ATOM	3444	O	GLY A 423	13.562	16.612	10.738	1.00	10.94	7
ATOM	3445	N	LEU A 424						
ATOM	3446	CA	LEU A 424						
ATOM	3447	CB	LEU A 424						
ATOM	3448	CG	LEU A 424						
ATOM	3449	CD	LEU A 424						
ATOM	3450	DD	LEU A 424						
ATOM	3451	O	LEU A 424						
ATOM	3452	N	ALA A 425						
ATOM	3453	CA	ALA A 425						
ATOM	3454	CB	ALA A 425						
ATOM	3455	CG	ALA A 425						
ATOM	3456	OG	ALA A 425						
ATOM	3457	C	ALA A 425						
ATOM	3458	O	ALA A 425						
ATOM	3459	N	ALA A 426						
ATOM	3460	CA	ALA A 426						
ATOM	3461	CB	ALA A 426						
ATOM	3462	CG	ALA A 426						
ATOM	3463	OG	ALA A 426						
ATOM	3464	C	ALA A 427						
ATOM	3465	O	ALA A 427						
ATOM	3466	N	LEU A 427						
ATOM	3467	CA	LEU A 427						
ATOM	3468	CB	LEU A 427						
ATOM	3469	CG	LEU A 427						
ATOM	3470	OG	LEU A 427						
ATOM	3471	C	LEU A 427						
ATOM	3472	O	LEU A 427						
ATOM	3473	N	ILE A 428						
ATOM	3474	CA	ILE A 428						
ATOM	3475	CB	ILE A 428						
ATOM	3476	CG	ILE A 428						
ATOM	3477	OG	ILE A 428						
ATOM	3478	C	ILE A 428						
ATOM	3479	O	ILE A 428						
ATOM	3480	N	THR A 429						
ATOM	3481	CA	THR A 429						
ATOM	3482	CB	THR A 429						
ATOM	3483	CG	THR A 429						
ATOM	3484	OG	THR A 429						
ATOM	3485	C	THR A 429						
ATOM	3486	O	THR A 429						
ATOM	3487	N	ASP A 430						
ATOM	3488	CA	ASP A 430						
ATOM	3489	CB	ASP A 430						
ATOM	3490	CG	ASP A 430						
ATOM	3491	OG	ASP A 430						
ATOM	3492	C	ASP A 430						
ATOM	3493	O	ASP A 430						
ATOM	3494	N	GLY A 431						
ATOM	3495	CA	GLY A 431						
ATOM	3496	C	GLY A 431						
ATOM	3497	O	GLY A 431						
ATOM	3498	N	PRO A 432						

ATOM	3499	CD	PRO A 432	35.409	10.665	0.884	1.00	14.46	6
ATOM	3500	CD	PRO A 432	33.653	11.935	-0.199	1.00	14.68	6
ATOM	3501	CB	PRO A 432	34.035	10.827	-1.190	1.00	14.46	6
ATOM	3502	CG	PRO A 432	35.224	10.168	-0.544	1.00	14.43	6
ATOM	3503	C	PRO A 432	32.163	11.902	-0.544	1.00	14.46	6
ATOM	3504	O	PRO A 432	31.795	11.354	1.273	1.00	14.84	8
ATOM	3505	N	GLY A 433	31.312	12.512	-0.641	1.00	15.15	7
ATOM	3506	CA	GLY A 433	29.882	12.569	-0.450	1.00	15.39	6
ATOM	3507	C	GLY A 433	29.192	11.254	-0.788	1.00	15.65	6
ATOM	3508	O	GLY A 433	29.816	10.259	-1.188	1.00	15.62	8
ATOM	3509	N	GLY A 434	27.885	11.213	-0.658	1.00	15.83	7
ATOM	3510	CA	GLY A 434	27.160	9.983	-0.950	1.00	15.94	6
ATOM	3511	C	GLY A 434	25.733	10.059	-0.444	1.00	15.96	6
ATOM	3512	O	GLY A 434	25.263	11.153	-0.176	1.00	16.25	8
ATOM	3513	N	ALA A 435	25.080	8.925	-0.297	1.00	15.72	7
ATOM	3514	CA	ALA A 435	23.722	8.072	0.128	1.00	15.72	6
ATOM	3515	C	ALA A 435	22.858	8.337	-1.047	1.00	15.08	6
ATOM	3516	C	ALA A 435	23.470	7.942	1.309	1.00	15.68	6
ATOM	3517	O	ALA A 435	24.260	7.007	1.516	1.00	15.51	8
ATOM	3518	N	LYS A 436	22.366	8.252	2.019	1.00	15.52	7
ATOM	3519	CA	LYS A 436	21.990	7.383	3.119	1.00	15.58	6
ATOM	3520	CG	LYS A 436	22.566	6.476	5.442	1.00	14.85	6
ATOM	3521	CG	LYS A 436	22.500	6.476	5.442	1.00	14.85	6
ATOM	3522	C	LYS A 436	23.071	6.769	6.810	1.00	13.83	6
ATOM	3523	CE	LYS A 436	24.448	7.441	6.784	1.00	12.21	6
ATOM	3524	N2	LYS A 436	25.498	6.400	6.652	1.00	11.33	7
ATOM	3525	C	LYS A 436	20.447	7.396	3.179	1.00	15.62	6
ATOM	3526	O	LYS A 436	19.778	8.405	3.060	1.00	15.33	8
ATOM	3527	N	ARG A 437	19.931	6.177	3.314	1.00	15.95	7
ATOM	3528	CA	ARG A 437	18.502	5.972	3.422	1.00	16.36	6
ATOM	3529	CG	ARG A 437	17.965	4.824	2.977	1.00	23.29	6
ATOM	3530	CG	ARG A 437	17.573	4.499	1.510	1.00	29.80	6
ATOM	3531	CD	ARG A 437	16.656	3.293	1.407	1.00	35.68	6
ATOM	3532	NE	ARG A 437	15.201	3.525	1.319	1.00	40.60	7
ATOM	3533	C2	ARG A 437	14.309	2.734	1.964	1.00	42.03	6
ATOM	3534	NH1	ARG A 437	14.735	1.740	2.755	1.00	42.08	7
ATOM	3535	NH2	ARG A 437	13.005	2.950	1.814	1.00	42.49	7
ATOM	3536	C	ARG A 437	18.202	6.050	4.911	1.00	15.94	6
ATOM	3537	O	ARG A 437	17.833	5.318	5.678	1.00	15.62	8
ATOM	3538	N	MET A 438	17.303	6.912	5.265	1.00	15.86	7
ATOM	3539	CA	MET A 438	17.019	7.059	6.722	1.00	15.87	6
ATOM	3540	CB	MET A 438	17.846	8.236	7.242	1.00	16.35	6
ATOM	3541	CG	MET A 438	19.360	8.200	7.266	1.00	15.99	6
ATOM	3542	SD	MET A 438	20.172	9.634	7.987	1.00	16.64	16
ATOM	3543	CE	MET A 438	19.698	10.989	6.970	1.00	14.67	6
ATOM	3544	C	MET A 438	15.525	7.205	6.983	1.00	15.63	6
ATOM	3545	O	MET A 438	14.774	7.662	6.109	1.00	15.49	8
ATOM	3546	N	TYR A 439	15.065	6.827	8.145	1.00	15.53	7
ATOM	3547	CA	TYR A 439	13.699	6.862	8.590	1.00	15.72	6
ATOM	3548	CB	TYR A 439	13.484	5.632	9.498	1.00	15.96	6
ATOM	3549	CG	TYR A 439	12.110	5.576	10.071	1.00	17.21	6
ATOM	3550	CD1	TYR A 439	11.044	5.338	9.188	1.00	17.52	6
ATOM	3551	CE1	TYR A 439	9.728	5.283	9.611	1.00	17.34	6
ATOM	3552	CD2	TYR A 439	11.815	5.768	11.397	1.00	16.76	6
ATOM	3553	CE2	TYR A 439	10.514	5.667	11.875	1.00	17.07	6
ATOM	3554	CZ	TYR A 439	9.490	5.433	10.974	1.00	17.36	6
ATOM	3555	OH	TYR A 439	8.184	5.345	11.408	1.00	17.36	8
ATOM	3556	C	TYR A 439	13.404	8.144	9.357	1.00	15.81	6
ATOM	3557	O	TYR A 439	13.994	8.512	10.382	1.00	15.50	8
ATOM	3558	N	VAL A 440	12.407	8.831	8.856	1.00	16.08	7
ATOM	3559	CA	VAL A 440	11.897	10.144	9.350	1.00	16.61	6
ATOM	3560	CB	VAL A 440	11.999	10.905	7.980	1.00	16.77	6
ATOM	3561	CG1	VAL A 440	10.764	11.601	7.561	1.00	17.08	6
ATOM	3562	CG2	VAL A 440	13.263	11.754	8.026	1.00	15.70	6
ATOM	3563	C	VAL A 440	10.554	10.106	10.031	1.00	17.07	6
ATOM	3564	O	VAL A 440	10.014	11.040	10.625	1.00	16.85	8
ATOM	3565	N	GLY A 441	9.900	8.915	9.995	1.00	17.47	7
ATOM	3566	CA	GLY A 441	8.607	8.729	10.597	1.00	18.13	6
ATOM	3567	C	GLY A 441	7.583	8.699	9.476	1.00	18.40	6
ATOM	3568	O	GLY A 441	7.616	9.450	8.514	1.00	18.47	8
ATOM	3569	N	ARG A 442	6.636	7.793	9.673	1.00	19.21	7
ATOM	3570	CA	ARG A 442	5.540	7.559	8.739	1.00	19.79	6
ATOM	3571	CB	ARG A 442	4.804	6.264	9.145	1.00	27.13	6
ATOM	3572	CG	ARG A 442	3.910	5.788	8.008	1.00	34.25	6
ATOM	3573	CD	ARG A 442	3.727	4.252	7.911	1.00	40.05	6
ATOM	3574	NE	ARG A 442	3.027	3.980	6.634	1.00	44.01	7
ATOM	3575	C2	ARG A 442	1.896	3.329	6.388	1.00	44.30	6
ATOM	3576	NH1	ARG A 442	1.175	2.772	7.381	1.00	47.10	7
ATOM	3577	NH2	ARG A 442	1.446	3.253	5.119	1.00	44.98	7
ATOM	3578	C	ARG A 442	4.586	8.725	8.657	1.00	19.53	6
ATOM	3579	O	ARG A 442	3.955	9.003	7.621	1.00	19.67	8
ATOM	3580	N	GLN A 443	4.479	9.544	9.684	1.00	19.05	7
ATOM	3581	CA	GLN A 443	3.607	10.709	9.658	1.00	18.69	6
ATOM	3582	CB	GLN A 443	3.431	11.246	11.093	1.00	21.29	6
ATOM	3583	CG	GLN A 443	4.808	11.675	11.634	1.00	23.26	6
ATOM	3584	CD	GLN A 443	5.581	10.603	12.390	1.00	24.64	6
ATOM	3585	OE1	GLN A 443	5.631	9.402	12.134	1.00	24.10	8
ATOM	3586	NE2	GLN A 443	6.316	11.066	13.438	1.00	25.50	7
ATOM	3587	C	GLN A 443	4.115	11.806	8.734	1.00	18.06	6
ATOM	3588	O	GLN A 443	3.414	12.798	8.501	1.00	17.90	8
ATOM	3589	N	ASN A 444	5.307	11.714	8.193	1.00	17.51	7
ATOM	3590	CA	ASN A 444	5.897	12.636	7.253	1.00	16.84	6
ATOM	3591	CB	ASN A 444	7.400	12.828	7.553	1.00	14.89	6
ATOM	3592	CG	ASN A 444	7.497	13.458	8.951	1.00	15.66	6
ATOM	3593	CD1	ASN A 444	6.765	14.374	9.269	1.00	13.70	8
ATOM	3594	ND2	ASN A 444	8.368	12.974	9.818	1.00	15.53	7
ATOM	3595	C	ASN A 444	5.814	12.078	5.820	1.00	16.45	6
ATOM	3596	O	ASN A 444	6.396	12.716	4.943	1.00	16.24	8
ATOM	3597	N	ALA A 445	5.196	10.917	5.640	1.00	16.01	7
ATOM	3598	CA	ALA A 445	5.075	10.268	4.365	1.00	16.03	6
ATOM	3599	CB	ALA A 445	4.109	9.075	4.403	1.00	15.55	6
ATOM	3600	C	ALA A 445	4.572	11.159	3.208	1.00	15.97	8
ATOM	3601	O	ALA A 445	3.626	11.896	3.441	1.00	15.97	6
ATOM	3602	N	GLY A 446	5.165	11.130	2.010	1.00	15.77	7
ATOM	3603	CA	GLY A 446	4.752	11.944	0.885	1.00	15.36	6
ATOM	3604	C	GLY A 446	5.207	13.378	0.863	1.00	15.20	6

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ATOM	3605	O	GLY A 446	4.924	14.124	-0.086	1.00	15.33	8
ATOM	3606	N	GLU A 447	5.963	13.897	1.827	1.00	14.73	7
ATOM	3607	C	GLU A 447	6.387	15.280	1.807	1.00	14.28	6
ATOM	3608	CB	GLU A 447	6.706	15.729	3.264	1.00	14.39	6
ATOM	3609	CG	GLU A 447	5.389	15.838	4.018	1.00	13.77	6
ATOM	3610	CD	GLU A 447	5.715	15.992	5.455	1.00	15.49	6
ATOM	3611	OE1	GLU A 447	6.875	16.135	5.959	1.00	15.55	8
ATOM	3612	OE2	GLU A 447	4.721	16.000	6.203	1.00	15.31	8
ATOM	3613	C	GLU A 447	7.644	15.680	1.041	1.00	13.72	6
ATOM	3614	O	GLU A 447	8.494	14.838	0.929	1.00	13.70	8
ATOM	3615	N	THR A 448	7.703	16.924	0.604	1.00	13.28	7
ATOM	3616	CA	THR A 448	8.904	17.386	-0.059	1.00	13.29	6
ATOM	3617	CB	THR A 448	8.681	18.432	-1.179	1.00	14.50	6
ATOM	3618	CG	THR A 448	7.898	17.829	-2.231	1.00	16.23	8
ATOM	3619	CD	THR A 448	9.966	18.972	-1.787	1.00	12.12	6
ATOM	3620	C	THR A 448	9.826	18.047	0.994	1.00	12.85	6
ATOM	3621	O	THR A 448	9.440	19.036	1.627	1.00	12.61	8
ATOM	3622	N	TRP A 449	11.021	17.500	1.176	1.00	12.53	7
ATOM	3623	CA	TRP A 449	12.011	18.069	2.095	1.00	12.56	6
ATOM	3624	CB	TRP A 449	12.564	16.992	3.035	1.00	9.33	6
ATOM	3625	CG	TRP A 449	11.619	16.660	4.133	1.00	9.67	6
ATOM	3626	CD	TRP A 449	10.762	15.974	5.402	1.00	8.65	6
ATOM	3627	CE2	TRP A 449	13.161	15.756	6.000	1.00	9.46	6
ATOM	3628	CE3	TRP A 449	10.237	16.787	4.154	1.00	9.60	6
ATOM	3629	NE1	TRP A 449	9.710	16.414	5.351	1.00	9.39	7
ATOM	3630	NE1	TRP A 449	10.730	15.465	7.438	1.00	9.93	6
ATOM	3631	CZ2	TRP A 449	13.135	15.216	7.286	1.00	7.79	6
ATOM	3632	CZ2	TRP A 449	11.953	15.068	7.958	1.00	8.43	6
ATOM	3633	C	TRP A 449	13.168	18.721	1.320	1.00	12.82	6
ATOM	3634	O	TRP A 449	13.563	18.178	0.275	1.00	12.56	8
ATOM	3635	N	HIS A 450	13.727	19.836	1.779	1.00	13.04	7
ATOM	3636	CA	HIS A 450	14.852	20.452	1.046	1.00	13.34	6
ATOM	3637	CB	HIS A 450	14.296	21.682	0.331	1.00	14.62	6
ATOM	3638	CG	HIS A 450	14.289	22.883	1.191	1.00	17.87	6
ATOM	3639	CD	HIS A 450	14.886	24.101	1.061	1.00	19.94	6
ATOM	3640	CE1	HIS A 450	13.580	22.945	2.378	1.00	20.15	7
ATOM	3641	CE1	HIS A 450	13.725	24.121	2.973	1.00	20.37	6
ATOM	3642	CE2	HIS A 450	14.513	24.848	2.189	1.00	21.15	7
ATOM	3643	CE2	HIS A 450	16.040	20.732	1.990	1.00	13.31	6
ATOM	3644	C	HIS A 450	15.781	20.891	3.188	1.00	13.10	8
ATOM	3645	O	HIS A 450	17.301	20.807	1.520	1.00	13.09	7
ATOM	3646	CA	ASP A 451	18.434	21.055	2.375	1.00	12.90	6
ATOM	3647	CB	ASP A 451	19.697	20.740	1.535	1.00	10.89	6
ATOM	3648	CG	ASP A 451	21.008	21.056	2.191	1.00	10.97	6
ATOM	3649	CD	ASP A 451	20.976	21.407	3.391	1.00	10.94	8
ATOM	3650	OE1	ASP A 451	22.111	20.978	1.592	1.00	11.53	8
ATOM	3651	OE2	ASP A 451	18.403	22.477	2.886	1.00	13.21	8
ATOM	3652	O	ASP A 451	18.643	23.419	2.089	1.00	13.23	8
ATOM	3653	N	ILE A 452	18.095	22.816	4.131	1.00	13.24	7
ATOM	3654	CA	ILE A 452	17.064	24.235	4.561	1.00	13.53	6
ATOM	3655	CB	ILE A 452	18.466	24.250	5.994	1.00	13.03	6
ATOM	3656	CG	ILE A 452	18.495	23.677	6.964	1.00	11.72	6
ATOM	3657	CD	ILE A 452						
ATOM	3658	CG1	ILE A 452	17.009	25.640	6.443	1.00	14.27	6
ATOM	3659	CD1	ILE A 452	16.275	25.551	7.802	1.00	14.37	6
ATOM	3660	C	ILE A 452	19.424	26.911	4.512	1.00	13.90	6
ATOM	3661	O	ILE A 452	19.482	26.166	4.529	1.00	13.78	8
ATOM	3662	N	THR A 453	20.598	24.254	4.476	1.00	14.31	7
ATOM	3663	CA	THR A 453	21.885	26.911	4.427	1.00	14.90	6
ATOM	3664	CB	THR A 453	23.063	23.977	4.697	1.00	12.74	6
ATOM	3665	CG1	THR A 453	23.194	23.019	3.614	1.00	12.38	8
ATOM	3666	CG2	THR A 453	22.905	23.215	6.001	1.00	12.32	6
ATOM	3667	C	THR A 453	22.184	25.480	3.030	1.00	15.80	6
ATOM	3668	O	THR A 453	23.073	26.280	2.774	1.00	15.75	8
ATOM	3669	N	GLY A 454	21.475	24.968	2.016	1.00	16.49	7
ATOM	3670	CA	GLY A 454	21.614	25.345	0.622	1.00	16.88	6
ATOM	3671	C	GLY A 454	22.752	24.598	-0.055	1.00	17.42	6
ATOM	3672	O	GLY A 454	22.967	24.858	-1.237	1.00	17.55	8
ATOM	3673	N	ASN A 455	23.496	23.700	0.568	1.00	17.75	7
ATOM	3674	CA	ASN A 455	24.590	22.992	-0.090	1.00	18.19	6
ATOM	3675	CB	ASN A 455	25.375	22.188	0.928	1.00	17.61	6
ATOM	3676	CG	ASN A 455	26.145	23.158	1.831	1.00	19.02	6
ATOM	3677	CD	ASN A 455	26.584	24.193	1.296	1.00	20.84	8
ATOM	3678	CE	ASN A 455	26.283	22.827	3.103	1.00	17.34	7
ATOM	3679	C	ASN A 455	24.050	22.108	-1.217	1.00	18.75	6
ATOM	3680	O	ASN A 455	24.847	21.968	-2.160	1.00	18.87	8
ATOM	3681	N	ARG A 456	22.843	21.544	-1.115	1.00	18.85	7
ATOM	3682	CA	ARG A 456	22.300	20.763	-2.215	1.00	19.42	6
ATOM	3683	CB	ARG A 456	22.051	19.313	-1.853	1.00	21.00	6
ATOM	3684	CG	ARG A 456	23.405	18.670	-1.612	1.00	22.06	6
ATOM	3685	CD	ARG A 456	23.079	17.230	-1.408	1.00	26.47	6
ATOM	3686	CE	ARG A 456	22.752	16.607	-2.676	1.00	27.86	7
ATOM	3687	CZ	ARG A 456	23.472	16.017	-3.613	1.00	29.09	6
ATOM	3688	NH1	ARG A 456	22.809	15.484	-4.631	1.00	29.42	7
ATOM	3689	NH2	ARG A 456	24.789	15.821	-3.652	1.00	30.25	7
ATOM	3690	C	ARG A 456	20.994	21.388	-2.721	1.00	19.69	6
ATOM	3691	O	ARG A 456	20.182	21.809	-1.881	1.00	19.86	8
ATOM	3692	N	SER A 457	20.777	21.515	-4.032	1.00	19.78	7
ATOM	3693	CA	SER A 457	19.533	22.134	-4.501	1.00	19.97	6
ATOM	3694	CB	SER A 457	19.748	23.040	-5.741	1.00	20.18	6
ATOM	3695	CG	SER A 457	20.301	22.068	-6.668	1.00	20.86	8
ATOM	3696	C	SER A 457	18.439	21.136	-4.883	1.00	19.94	6
ATOM	3697	O	SER A 457	17.317	21.592	-5.183	1.00	20.17	8
ATOM	3698	N	GLU A 458	18.708	19.841	-4.835	1.00	19.72	7
ATOM	3699	CA	GLU A 458	17.687	18.883	-5.161	1.00	19.82	6
ATOM	3700	CB	GLU A 458	18.321	17.611	-5.803	1.00	24.71	6
ATOM	3701	CG	GLU A 458	17.134	17.001	-6.543	1.00	31.90	6
ATOM	3702	CD	GLU A 458	17.152	15.635	-7.168	1.00	36.18	6
ATOM	3703	OE1	GLU A 458	18.250	15.229	-7.481	1.00	38.60	8
ATOM	3704	OE2	GLU A 458	16.057	14.979	-7.142	1.00	38.01	8
ATOM	3705	C	GLU A 458	16.850	18.407	-3.978	1.00	19.28	6
ATOM	3706	O	GLU A 458	17.375	17.778	-3.068	1.00	19.23	8
ATOM	3707	N	PRO A 459	15.545	18.628	-4.028	1.00	18.75	7
ATOM	3708	CA	PRO A 459	14.893	19.401	-5.083	1.00	18.49	6
ATOM	3709	CB	PRO A 459	14.611	18.231	-2.974	1.00	18.56	6
ATOM	3710	CD	PRO A 459	13.270	18.916	-3.298	1.00	18.40	6

ATOM	3711	CG	PRO A 459	13.637	19.885	-4.393	1.00	18.37	6	ATOM	3764	CA	TRP A 467	11.860	6.686	4.486	1.00	20.35	6
ATOM	3712	C	PRO A 459	14.504	16.723	-2.839	1.00	18.47	6	ATOM	3765	CB	TRP A 467	12.439	5.313	4.107	1.00	20.44	6
ATOM	3713	O	PRO A 459	14.829	15.979	-3.780	1.00	18.68	8	ATOM	3766	CG	TRP A 467	12.372	4.283	5.181	1.00	20.04	6
ATOM	3714	H	VAL A 460	14.113	16.146	-1.728	1.00	18.24	7	ATOM	3767	CD2	TRP A 467	13.427	3.771	5.993	1.00	19.41	6
ATOM	3715	CA	VAL A 460	13.987	14.691	-1.504	1.00	18.19	6	ATOM	3768	CE2	TRP A 467	12.844	2.826	6.880	1.00	19.61	6
ATOM	3716	CB	VAL A 460	14.906	14.168	-0.379	1.00	17.56	6	ATOM	3769	CE3	TRP A 467	14.803	3.987	6.049	1.00	18.58	6
ATOM	3717	CG1	VAL A 460	14.739	12.685	-0.076	1.00	17.48	6	ATOM	3770	CD1	TRP A 467	11.227	3.633	5.591	1.00	20.26	6
ATOM	3718	CG2	VAL A 460	16.371	14.396	-0.750	1.00	17.31	6	ATOM	3771	NE1	TRP A 467	11.497	2.779	6.622	1.00	19.67	7
ATOM	3719	C	VAL A 460	12.528	14.396	-1.209	1.00	18.23	6	ATOM	3772	CD2	TRP A 467	13.593	2.102	7.824	1.00	19.59	6
ATOM	3720	O	VAL A 460	11.892	15.157	-0.428	1.00	18.51	8	ATOM	3773	CD3	TRP A 467	15.552	3.268	6.997	1.00	20.04	6
ATOM	3721	H	VAL A 461	11.894	13.362	-1.798	1.00	18.03	7	ATOM	3774	CH2	TRP A 467	14.959	2.315	7.868	1.00	19.86	6
ATOM	3722	CA	VAL A 461	10.468	13.105	-1.458	1.00	17.66	6	ATOM	3775	C	TRP A 467	12.174	7.631	3.312	1.00	20.06	6
ATOM	3723	CB	VAL A 461	9.584	12.863	-2.709	1.00	17.06	6	ATOM	3776	O	TRP A 467	11.355	7.837	2.413	1.00	19.99	8
ATOM	3724	CG1	VAL A 461	8.143	12.564	-2.256	1.00	16.42	6	ATOM	3777	H	GLY A 468	13.356	8.193	3.372	1.00	19.55	7
ATOM	3725	CG2	VAL A 461	9.629	14.023	-3.678	1.00	15.12	6	ATOM	3778	CA	GLY A 468	13.838	9.105	2.345	1.00	19.08	6
ATOM	3726	C	VAL A 461	10.418	11.943	-0.456	1.00	17.45	6	ATOM	3779	O	GLY A 468	15.293	8.667	2.044	1.00	18.51	8
ATOM	3727	O	VAL A 461	11.046	10.893	-0.596	1.00	17.01	8	ATOM	3780	O	GLY A 468	15.969	8.121	2.908	1.00	18.42	7
ATOM	3728	H	ILE A 462	9.707	12.111	0.647	1.00	17.69	7	ATOM	3781	N	GLU A 469	15.761	8.896	0.848	1.00	18.42	7
ATOM	3729	CA	ILE A 462	9.596	11.050	1.642	1.00	18.12	6	ATOM	3782	CA	GLU A 469	17.153	8.577	0.487	1.00	18.35	6
ATOM	3730	CB	ILE A 462	9.212	11.549	3.046	1.00	15.81	6	ATOM	3783	CB	GLU A 469	17.287	7.714	-0.771	1.00	23.55	6
ATOM	3731	CG1	ILE A 462	9.222	10.334	3.984	1.00	15.11	6	ATOM	3784	CG	GLU A 469	18.710	7.626	-1.293	1.00	29.59	6
ATOM	3732	CG2	ILE A 462	10.089	12.691	3.597	1.00	13.00	6	ATOM	3785	CG	GLU A 469	18.967	7.178	-2.729	1.00	34.28	6
ATOM	3733	CO1	ILE A 462	11.575	12.439	3.462	1.00	9.27	6	ATOM	3786	OE1	GLU A 469	19.831	6.252	-2.904	1.00	36.09	8
ATOM	3734	C	ILE A 462	8.554	10.036	1.116	1.00	18.85	6	ATOM	3787	OE2	GLU A 469	18.340	7.755	-3.681	1.00	35.52	8
ATOM	3735	O	ILE A 462	7.432	10.390	0.717	1.00	18.67	8	ATOM	3788	C	GLU A 469	17.805	9.964	0.424	1.00	17.57	6
ATOM	3736	H	ASN A 463	8.922	8.755	1.138	1.00	19.55	7	ATOM	3789	O	GLU A 469	17.555	10.801	-0.433	1.00	17.46	8
ATOM	3737	CA	ASN A 463	8.090	7.650	0.672	1.00	20.49	6	ATOM	3790	N	PHE A 470	18.666	10.297	1.388	1.00	17.09	7
ATOM	3738	CB	ASN A 463	8.960	6.443	0.342	1.00	20.20	6	ATOM	3791	CA	PHE A 470	19.246	11.640	1.415	1.00	16.47	6
ATOM	3739	CG	ASN A 463	9.411	5.430	1.361	1.00	21.59	6	ATOM	3792	CB	PHE A 470	19.076	12.181	2.850	1.00	14.77	6
ATOM	3740	CO1	ASN A 463	9.117	5.376	2.570	1.00	22.11	8	ATOM	3793	CG	PHE A 470	17.686	12.126	3.451	1.00	11.90	6
ATOM	3741	HO2	ASN A 463	10.221	4.455	0.904	1.00	22.11	7	ATOM	3794	CD1	PHE A 470	17.301	11.041	4.208	1.00	11.90	6
ATOM	3742	C	ASN A 463	6.975	7.297	1.630	1.00	21.45	6	ATOM	3795	CD2	PHE A 470	16.823	13.197	3.296	1.00	10.16	6
ATOM	3743	O	ASN A 463	6.884	7.762	2.770	1.00	21.42	8	ATOM	3796	CE1	PHE A 470	16.037	11.030	4.790	1.00	11.36	6
ATOM	3744	H	SER A 464	6.070	6.390	1.173	1.00	22.31	7	ATOM	3797	CE2	PHE A 470	15.562	13.155	3.871	1.00	9.61	6
ATOM	3745	CA	SER A 464	4.877	5.971	1.916	1.00	22.97	6	ATOM	3798	CZ	PHE A 470	15.159	12.069	4.605	1.00	9.27	6
ATOM	3746	CB	SER A 464	3.915	5.159	1.024	1.00	23.92	6	ATOM	3799	C	PHE A 470	20.682	11.731	0.945	1.00	16.14	6
ATOM	3747	CG	SER A 464	4.365	3.841	0.731	1.00	25.69	8	ATOM	3800	O	PHE A 470	21.406	10.761	1.154	1.00	16.37	8
ATOM	3748	C	SER A 464	5.187	5.303	3.248	1.00	23.29	6	ATOM	3801	N	HIS A 471	21.142	12.807	0.363	1.00	15.78	7
ATOM	3749	O	SER A 464	4.319	5.400	4.131	1.00	23.52	8	ATOM	3802	CA	HIS A 471	22.462	13.007	-0.146	1.00	15.69	6
ATOM	3750	H	GLU A 465	6.344	4.722	3.486	1.00	23.46	7	ATOM	3803	CB	HIS A 471	22.332	13.373	-1.655	1.00	17.00	6
ATOM	3751	CA	GLU A 465	6.814	4.134	4.708	1.00	23.73	6	ATOM	3804	CG	HIS A 471	21.894	12.216	-2.515	1.00	20.58	6
ATOM	3752	CB	GLU A 465	7.931	3.164	4.313	1.00	29.98	6	ATOM	3805	CD2	HIS A 471	22.588	11.406	-3.372	1.00	21.49	6
ATOM	3753	CG	GLU A 465	7.852	1.671	4.515	1.00	35.99	6	ATOM	3806	HO1	HIS A 471	20.560	11.780	-2.567	1.00	22.05	7
ATOM	3754	CO	GLU A 465	6.562	1.117	3.976	1.00	39.49	6	ATOM	3807	CE1	HIS A 471	20.481	10.745	-3.399	1.00	21.74	6
ATOM	3755	OE1	GLU A 465	6.407	1.177	2.734	1.00	41.43	8	ATOM	3808	WE2	HIS A 471	21.688	10.491	-3.900	1.00	22.49	7
ATOM	3756	OE2	GLU A 465	5.709	0.684	4.812	1.00	41.76	8	ATOM	3809	C	HIS A 471	23.282	14.111	0.945	1.00	15.47	6
ATOM	3757	C	GLU A 465	7.511	5.095	5.721	1.00	23.27	6	ATOM	3810	O	HIS A 471	22.727	15.102	0.997	1.00	15.28	8
ATOM	3758	O	GLU A 465	7.857	4.672	6.848	1.00	23.24	8	ATOM	3811	N	VAL A 472	24.618	13.993	0.446	1.00	15.23	7
ATOM	3759	H	GLY A 466	7.744	6.345	5.324	1.00	22.53	7	ATOM	3812	CA	VAL A 472	25.529	14.978	0.964	1.00	15.01	6
ATOM	3760	CA	GLY A 466	8.436	7.317	6.135	1.00	21.95	6	ATOM	3813	CB	VAL A 472	26.385	14.698	2.271	1.00	16.48	6
ATOM	3761	C	GLY A 466	9.969	7.245	5.909	1.00	21.47	6	ATOM	3814	CG1	VAL A 472	26.201	15.727	3.368	1.00	15.07	6
ATOM	3762	O	GLY A 466	10.728	7.644	6.820	1.00	21.33	8	ATOM	3815	CG2	VAL A 472	26.275	13.274	2.750	1.00	17.23	6
ATOM	3763	N	TRP A 467	10.441	6.770	4.751	1.00	20.79	7	ATOM	3816	C	VAL A 472	26.730	15.205	0.001	1.00	14.42	6

ATOM	3817	O	VAL A 472	27.266	14.169	-0.462	1.00	14.29	8
ATOM	3818	H	ASH A 473	27.200	16.444	-0.101	1.00	13.78	7
ATOM	3819	CA	ASH A 473	28.404	16.662	-0.901	1.00	13.30	6
ATOM	3820	CB	ASH A 473	28.514	18.108	-1.339	1.00	13.44	6
ATOM	3821	CG	ASH A 473	27.403	18.519	-2.301	1.00	15.11	6
ATOM	3822	CD	ASH A 473	26.781	17.637	-2.882	1.00	15.07	6
ATOM	3823	ND2	ASH A 473	27.148	19.805	-2.494	1.00	15.52	7
ATOM	3824	C	ASH A 473	29.633	16.278	-0.086	1.00	12.99	6
ATOM	3825	O	ASH A 473	29.567	16.164	-1.139	1.00	12.88	6
ATOM	3826	H	GLY A 474	30.792	16.066	-0.723	1.00	12.57	7
ATOM	3827	CA	GLY A 474	32.004	15.690	0.026	1.00	11.90	6
ATOM	3828	C	GLY A 474	32.429	16.874	0.897	1.00	11.47	6
ATOM	3829	D	GLY A 474	32.305	18.054	0.524	1.00	11.68	8
ATOM	3830	H	GLY A 475	32.940	16.534	2.058	1.00	10.93	7
ATOM	3831	CA	GLY A 475	33.425	17.392	3.139	1.00	10.37	6
ATOM	3832	C	GLY A 475	32.350	18.425	3.486	1.00	10.04	6
ATOM	3833	O	GLY A 475	32.666	19.606	3.607	1.00	9.82	8
ATOM	3834	H	SER A 476	31.076	17.953	3.556	1.00	9.71	7
ATOM	3835	CA	SER A 476	29.330	19.038	2.348	1.00	10.16	6
ATOM	3836	CB	SER A 476	28.487	20.170	2.237	1.00	11.03	8
ATOM	3837	OG	SER A 476	28.910	18.374	4.718	1.00	8.97	6
ATOM	3838	C	SER A 476	28.982	17.301	5.311	1.00	8.60	8
ATOM	3839	O	SER A 476	27.865	19.207	6.864	1.00	8.73	7
ATOM	3840	H	VAL A 477	26.711	18.975	5.699	1.00	8.62	6
ATOM	3841	CA	VAL A 477	26.705	19.802	7.028	1.00	6.94	6
ATOM	3842	CB	VAL A 477	26.953	21.201	6.811	1.00	5.00	6
ATOM	3843	CG1	VAL A 477	25.389	19.640	7.754	1.00	5.67	6
ATOM	3844	CG2	VAL A 477	25.462	19.333	4.887	1.00	8.35	6
ATOM	3845	C	VAL A 477	25.485	20.297	4.139	1.00	8.26	8
ATOM	3846	O	VAL A 477	24.403	18.567	5.033	1.00	8.45	7
ATOM	3847	H	SER A 478	23.087	18.761	4.462	1.00	8.36	6
ATOM	3848	CA	SER A 478	22.792	17.840	3.254	1.00	8.85	6
ATOM	3849	CB	SER A 478	23.251	18.520	2.073	1.00	11.98	8
ATOM	3850	OG	SER A 478	22.074	18.493	5.574	1.00	8.16	6
ATOM	3851	C	SER A 478	22.161	17.527	6.326	1.00	7.79	8
ATOM	3852	O	SER A 478	21.114	19.406	5.720	1.00	8.43	7
ATOM	3853	H	ILE A 479	20.039	19.323	6.693	1.00	8.49	6
ATOM	3854	CA	ILE A 479	20.160	20.274	7.894	1.00	8.78	6
ATOM	3855	CB	ILE A 479	18.976	19.999	8.846	1.00	8.48	6
ATOM	3856	CG2	ILE A 479	21.502	20.102	8.647	1.00	8.82	6
ATOM	3857	CG1	ILE A 479	21.914	21.342	9.399	1.00	7.53	6
ATOM	3858	CD1	ILE A 479	18.689	19.539	6.015	1.00	8.75	6
ATOM	3859	C	ILE A 479	18.346	20.671	5.734	1.00	8.74	8
ATOM	3860	O	ILE A 479	17.969	18.447	5.791	1.00	9.32	7
ATOM	3861	H	THR A 480	16.682	18.457	5.143	1.00	10.04	6
ATOM	3862	CA	THR A 480	16.431	17.093	4.465	1.00	10.47	6
ATOM	3863	CB	THR A 480	17.358	16.901	3.299	1.00	11.51	6
ATOM	3864	CG	THR A 480	18.620	16.314	3.605	1.00	12.15	6
ATOM	3865	CD1	THR A 480	19.531	16.102	2.589	1.00	12.53	6
ATOM	3866	CE1	THR A 480	17.080	17.306	2.091	1.00	11.63	6
ATOM	3867	CE2	THR A 480	17.988	17.112	0.996	1.00	12.21	6
ATOM	3868	CE2	THR A 480	19.177	16.496	1.294	1.00	12.89	6
ATOM	3869	CZ	THR A 480						
ATOM	3870	OH	THR A 480						
ATOM	3871	C	THR A 480						
ATOM	3872	O	THR A 480						
ATOM	3873	H	VAL A 481						
ATOM	3874	CA	VAL A 481						
ATOM	3875	CB	VAL A 481						
ATOM	3876	CG1	VAL A 481						
ATOM	3877	CG2	VAL A 481						
ATOM	3878	C	VAL A 481						
ATOM	3879	O	VAL A 481						
ATOM	3880	H	GLM A 482						
ATOM	3881	CA	GLM A 482						
ATOM	3882	CB	GLM A 482						
ATOM	3883	CG	GLM A 482						
ATOM	3884	CD	GLM A 482						
ATOM	3885	OE1	GLM A 482						
ATOM	3886	NE2	GLM A 482						
ATOM	3887	C	GLM A 482						
ATOM	3888	O	GLM A 482						
ATOM	3889	H	ARG A 483						
ATOM	3890	CA	ARG A 483						
ATOM	3891	CB	ARG A 483						
ATOM	3892	CG	ARG A 483						
ATOM	3893	CD	ARG A 483						
ATOM	3894	NE	ARG A 483						
ATOM	3895	CZ	ARG A 483						
ATOM	3896	WH1	ARG A 483						
ATOM	3897	WH2	ARG A 483						
ATOM	3898	C	ARG A 483						
ATOM	3899	O	ARG A 483						
ATOM	3900	OT	ARG A 483						
ATOM	3901	CA	ILM \$ 501						
ATOM	3902	CA	ILM \$ 502						
ATOM	3903	CA	ILM \$ 503						
ATOM	3904	CA	ILM \$ 504						
ATOM	3905	OW1	WAT X 1						
ATOM	3906	OW2	WAT X 1						
ATOM	3907	OW3	WAT X 1						
ATOM	3908	OW4	WAT X 1						
ATOM	3909	OW5	WAT X 1						
ATOM	3910	OW6	WAT X 1						
ATOM	3911	OW7	WAT X 1						
ATOM	3912	OW8	WAT X 1						
ATOM	3913	OW9	WAT X 1						
ATOM	3914	OW0	WAT X 2						
ATOM	3915	OW1	WAT X 2						
ATOM	3916	OW2	WAT X 2						
ATOM	3917	OW3	WAT X 2						
ATOM	3918	OW4	WAT X 2						
ATOM	3919	OW5	WAT X 2						
ATOM	3920	OW6	WAT X 2						
ATOM	3921	OW7	WAT X 2						
ATOM	3922	OW8	WAT X 2						

ATOM	3923	OM9	WAT	X	2	42.991	28.597	56.879	1.00	19.54	8
ATOM	3924	OM0	WAT	X	3	42.416	33.909	17.726	1.00	10.85	8
ATOM	3925	OM1	WAT	X	3	48.842	22.953	44.340	1.00	7.66	8
ATOM	3926	OM2	WAT	X	3	36.038	55.628	43.083	1.00	10.34	8
ATOM	3927	OM3	WAT	X	3	58.570	25.578	42.683	1.00	12.51	8
ATOM	3928	OM4	WAT	X	3	35.732	43.524	49.882	1.00	5.95	8
ATOM	3929	OM5	WAT	X	3	26.190	18.692	1.154	1.00	12.57	8
ATOM	3930	OM6	WAT	X	3	40.723	25.525	46.044	1.00	10.44	8
ATOM	3931	OM7	WAT	X	3	41.640	28.398	45.135	1.00	5.00	8
ATOM	3932	OM8	WAT	X	3	36.546	42.416	33.352	1.00	5.00	8
ATOM	3933	OM9	WAT	X	3	40.987	21.110	52.091	1.00	20.54	8
ATOM	3934	OM0	WAT	X	4	37.695	27.410	12.493	1.00	11.34	8
ATOM	3935	OM1	WAT	X	4	22.844	23.707	36.872	1.00	9.80	8
ATOM	3936	OM2	WAT	X	4	36.012	18.648	48.284	1.00	17.35	8
ATOM	3937	OM3	WAT	X	4	31.899	45.870	33.523	1.00	10.56	8
ATOM	3938	OM4	WAT	X	4	30.501	38.096	33.954	1.00	11.67	8
ATOM	3939	OM5	WAT	X	4	22.073	12.907	32.231	1.00	10.97	8
ATOM	3940	OM6	WAT	X	4	40.468	14.451	42.396	1.00	12.74	8
ATOM	3941	OM7	WAT	X	4	53.405	37.236	44.839	1.00	12.00	8
ATOM	3942	OM8	WAT	X	4	43.396	20.817	52.968	1.00	25.21	8
ATOM	3943	OM9	WAT	X	4	45.712	34.753	17.330	1.00	22.47	8
ATOM	3944	OM0	WAT	X	5	52.299	25.204	54.738	1.00	18.85	8
ATOM	3945	OM1	WAT	X	5	10.464	19.211	8.671	1.00	8.04	8
ATOM	3946	OM2	WAT	X	5	23.407	21.100	30.729	1.00	15.19	8
ATOM	3947	OM3	WAT	X	5	34.672	39.007	47.914	1.00	25.93	8
ATOM	3948	OM4	WAT	X	5	39.440	24.513	6.213	1.00	20.60	8
ATOM	3949	OM5	WAT	X	5	43.207	54.381	40.149	1.00	23.71	8
ATOM	3950	OM6	WAT	X	5	29.887	49.393	26.775	1.00	10.08	8
ATOM	3951	OM7	WAT	X	5	18.296	28.320	27.646	1.00	17.61	8
ATOM	3952	OM8	WAT	X	5	42.657	37.701	31.679	1.00	16.67	8
ATOM	3953	OM9	WAT	X	5	43.242	40.411	24.206	1.00	19.05	8
ATOM	3954	OM0	WAT	X	6	27.361	18.395	39.419	1.00	14.74	8
ATOM	3955	OM1	WAT	X	6	28.339	52.900	35.976	1.00	18.51	8
ATOM	3956	OM2	WAT	X	6	37.756	14.989	39.100	1.00	17.01	8
ATOM	3957	OM3	WAT	X	6	22.840	21.238	35.474	1.00	13.60	8
ATOM	3958	OM4	WAT	X	6	38.940	13.232	9.026	1.00	11.51	8
ATOM	3959	OM5	WAT	X	6	25.342	16.185	20.356	1.00	18.86	8
ATOM	3960	OM6	WAT	X	6	8.361	17.329	8.642	1.00	13.52	8
ATOM	3961	OM7	WAT	X	6	37.794	6.917	7.269	1.00	20.73	8
ATOM	3962	OM8	WAT	X	6	45.060	49.979	33.793	1.00	12.44	8
ATOM	3963	OM9	WAT	X	6	36.427	41.328	48.308	1.00	11.02	8
ATOM	3964	OM0	WAT	X	7	41.263	15.827	37.266	1.00	22.49	8
ATOM	3965	OM1	WAT	X	7	25.131	39.394	49.866	1.00	10.30	8
ATOM	3966	OM2	WAT	X	7	51.050	21.873	54.397	1.00	18.11	8
ATOM	3967	OM3	WAT	X	7	43.851	40.827	26.978	1.00	36.82	8
ATOM	3968	OM4	WAT	X	7	48.952	26.479	52.035	1.00	17.95	8
ATOM	3969	OM5	WAT	X	7	24.717	49.514	27.044	1.00	19.57	8
ATOM	3970	OM6	WAT	X	7	32.551	52.703	28.488	1.00	9.04	8
ATOM	3971	OM7	WAT	X	7	44.885	26.009	54.445	1.00	7.24	8
ATOM	3972	OM8	WAT	X	7	38.325	36.644	45.393	1.00	19.65	8
ATOM	3973	OM9	WAT	X	7	21.609	12.965	20.907	1.00	9.32	8
ATOM	3974	OM0	WAT	X	8	24.711	13.545	20.784	1.00	23.06	8
ATOM	3975	OM1	WAT	X	8	42.374	43.789	25.824	1.00	28.85	8
ATOM	3976	OM2	WAT	X	8	18.586	45.140	20.306	1.00	24.89	8
ATOM	3977	OM3	WAT	X	8	40.969	25.117	33.960	1.00	19.79	8
ATOM	3978	OM4	WAT	X	8	20.088	43.470	17.087	1.00	16.72	8
ATOM	3979	OM5	WAT	X	8	38.467	37.011	11.354	1.00	25.51	8
ATOM	3980	OM6	WAT	X	8	13.729	9.292	-1.198	1.00	18.29	8
ATOM	3981	OM7	WAT	X	8	37.082	34.587	46.550	1.00	20.44	8
ATOM	3982	OM8	WAT	X	8	33.674	28.739	26.941	1.00	37.20	8
ATOM	3983	OM9	WAT	X	8	44.040	39.609	29.378	1.00	15.09	8
ATOM	3984	OM0	WAT	X	9	5.980	17.940	10.956	1.00	15.78	8
ATOM	3985	OM1	WAT	X	9	37.928	39.774	25.743	1.00	20.89	8
ATOM	3986	OM2	WAT	X	9	30.894	54.048	35.873	1.00	15.39	8
ATOM	3987	OM3	WAT	X	9	28.071	34.048	54.110	1.00	17.12	8
ATOM	3988	OM4	WAT	X	9	18.742	28.715	32.238	1.00	16.32	8
ATOM	3989	OM5	WAT	X	9	21.957	31.164	51.343	1.00	17.53	8
ATOM	3990	OM6	WAT	X	9	17.533	31.407	37.350	1.00	18.05	8
ATOM	3991	OM7	WAT	X	9	33.329	26.312	6.343	1.00	16.49	8
ATOM	3992	OM8	WAT	X	9	52.348	36.436	42.429	1.00	22.51	8
ATOM	3993	OM9	WAT	X	9	33.954	32.866	59.563	1.00	24.70	8
ATOM	3994	OM0	WAT	X	10	20.209	19.419	22.073	1.00	15.65	8
ATOM	3995	OM1	WAT	X	10	32.236	16.522	47.616	1.00	20.65	8
ATOM	3996	OM2	WAT	X	10	38.512	27.238	32.842	1.00	17.87	8
ATOM	3997	OM3	WAT	X	10	29.117	21.774	-1.117	1.00	25.65	8
ATOM	3998	OM4	WAT	X	10	36.476	40.547	18.282	1.00	25.86	8
ATOM	3999	OM5	WAT	X	10	18.917	5.144	16.972	1.00	16.17	8
ATOM	4000	OM6	WAT	X	10	23.106	43.383	45.060	1.00	22.47	8
ATOM	4001	OM7	WAT	X	10	27.983	24.700	5.027	1.00	20.60	8
ATOM	4002	OM8	WAT	X	10	34.986	39.869	15.784	1.00	23.70	8
ATOM	4003	OM9	WAT	X	10	5.987	15.831	-1.902	1.00	32.41	8
ATOM	4004	OM0	WAT	X	11	19.643	16.427	-2.512	1.00	35.14	8
ATOM	4005	OM1	WAT	X	11	17.172	19.237	19.672	1.00	29.78	8
ATOM	4006	OM2	WAT	X	11	49.760	21.003	51.233	1.00	9.95	8
ATOM	4007	OM3	WAT	X	11	41.639	31.412	35.004	1.00	25.82	8
ATOM	4008	OM4	WAT	X	11	25.364	51.628	41.093	1.00	29.63	8
ATOM	4009	OM5	WAT	X	11	19.805	23.778	36.990	1.00	33.98	8
ATOM	4010	OM6	WAT	X	11	42.937	27.882	12.460	1.00	37.03	8
ATOM	4011	OM7	WAT	X	11	18.451	29.166	35.333	1.00	27.81	8
ATOM	4012	OM8	WAT	X	11	24.969	26.021	50.840	1.00	26.74	8
ATOM	4013	OM9	WAT	X	11	43.160	54.157	43.072	1.00	23.83	8
ATOM	4014	OM0	WAT	X	12	12.642	37.968	31.162	1.00	65.20	8
ATOM	4015	OM1	WAT	X	12	32.411	23.218	5.138	1.00	18.08	8
ATOM	4016	OM2	WAT	X	12	19.308	3.707	13.407	1.00	50.55	8
ATOM	4017	OM3	WAT	X	12	17.400	20.494	-1.396	1.00	25.22	8
ATOM	4018	OM4	WAT	X	12	38.504	40.778	36.668	1.00	40.52	8
ATOM	4019	OM5	WAT	X	12	46.693	16.740	48.249	1.00	22.77	8
ATOM	4020	OM6	WAT	X	12	44.237	51.654	41.807	1.00	30.69	8
ATOM	4021	OM7	WAT	X	12	29.593	23.052	4.777	1.00	24.15	8
ATOM	4022	OM8	WAT	X	12	25.325	25.894	6.415	1.00	23.43	8
ATOM	4023	OM9	WAT	X	12	37.028	10.496	27.680	1.00	13.65	8
ATOM	4024	OM0	WAT	X	13	15.428	33.267	21.245	1.00	27.08	8
ATOM	4025	OM1	WAT	X	13	32.665	39.080	54.672	1.00	21.60	8
ATOM	4026	OM2	WAT	X	13	46.251	40.891	31.602	1.00	25.79	8
ATOM	4027	OM3	WAT	X	13	38.486	30.224	30.783	1.00	20.87	8
ATOM	4028	OM4	WAT	X	13	42.551	46.583	21.900	1.00	28.42	8

ATOM	4029	045	WAT	X	13	13.009	12.182	-4.067	1.00	27.61	8
ATOM	4030	046	WAT	X	13	32.756	8.582	1.824	1.00	29.04	8
ATOM	4031	047	WAT	X	13	16.249	23.415	-2.919	1.00	36.05	8
ATOM	4032	048	WAT	X	13	36.916	46.802	51.068	1.00	13.92	8
ATOM	4033	049	WAT	X	13	51.456	45.867	33.043	1.00	27.25	8
ATOM	4034	040	WAT	X	14	44.576	23.979	15.915	1.00	39.18	8
ATOM	4035	041	WAT	X	14	16.346	4.264	16.031	1.00	22.00	8
ATOM	4036	042	WAT	X	14	32.347	13.546	-3.049	1.00	37.27	8
ATOM	4037	043	WAT	X	14	45.366	38.058	33.758	1.00	20.30	8
ATOM	4038	044	WAT	X	14	4.549	18.600	33.099	1.00	20.90	8
ATOM	4039	045	WAT	X	14	15.354	36.796	43.569	1.00	18.79	8
ATOM	4040	046	WAT	X	14	44.963	30.462	57.791	1.00	33.45	8
ATOM	4041	047	WAT	X	14	53.136	23.195	37.475	1.00	31.43	8
ATOM	4042	048	WAT	X	14	30.694	15.659	-3.842	1.00	23.59	8
ATOM	4043	049	WAT	X	14	39.010	7.257	14.525	1.00	37.98	8
ATOM	4044	040	WAT	X	15	37.498	55.360	32.899	1.00	35.04	8
ATOM	4045	041	WAT	X	15	21.133	44.448	35.481	1.00	35.84	8
ATOM	4046	042	WAT	X	15	23.993	4.153	14.519	1.00	20.07	8
ATOM	4047	043	WAT	X	15	21.568	23.231	44.662	1.00	34.60	8
ATOM	4048	044	WAT	X	15	9.185	24.444	6.708	1.00	19.79	8
ATOM	4049	045	WAT	X	15	44.586	35.812	31.349	1.00	48.30	8
ATOM	4050	046	WAT	X	15	30.789	25.745	52.371	1.00	38.63	8
ATOM	4051	047	WAT	X	15	41.284	38.972	11.403	1.00	29.22	8
ATOM	4052	048	WAT	X	15	56.979	36.187	58.016	1.00	37.19	8
ATOM	4053	049	WAT	X	15	25.886	5.827	3.524	1.00	21.64	8
ATOM	4054	040	WAT	X	16	41.689	14.341	39.346	1.00	28.91	8
ATOM	4055	041	WAT	X	16	20.238	10.905	31.899	1.00	29.69	8
ATOM	4056	042	WAT	X	16	44.542	44.756	52.978	1.00	18.83	8
ATOM	4057	043	WAT	X	16	57.377	17.228	51.604	1.00	20.62	8
ATOM	4058	044	WAT	X	16	33.851	33.580	56.957	1.00	22.46	8
ATOM	4059	045	WAT	X	16	35.776	25.007	52.963	1.00	30.96	8
ATOM	4060	046	WAT	X	16	50.697	26.378	37.894	1.00	17.69	8
ATOM	4061	047	WAT	X	16	35.244	16.237	47.346	1.00	35.92	8
ATOM	4062	048	WAT	X	16	41.297	31.972	30.043	1.00	23.15	8
ATOM	4063	049	WAT	X	16	60.104	21.780	53.887	1.00	24.69	8
ATOM	4064	040	WAT	X	17	33.930	36.911	56.317	1.00	28.54	8
ATOM	4065	041	WAT	X	17	27.783	49.620	50.985	1.00	21.73	8
ATOM	4066	042	WAT	X	17	38.322	12.309	23.483	1.00	42.93	8
ATOM	4067	043	WAT	X	17	19.759	16.587	26.896	1.00	25.91	8
ATOM	4068	044	WAT	X	17	18.392	24.561	-0.866	1.00	45.44	8
ATOM	4069	045	WAT	X	17	43.370	16.553	29.268	1.00	24.28	8
ATOM	4070	046	WAT	X	17	12.508	25.520	4.810	1.00	39.21	8
ATOM	4071	047	WAT	X	17	44.009	35.484	9.586	1.00	27.73	8
ATOM	4072	048	WAT	X	17	38.155	15.958	4.049	1.00	24.72	8
ATOM	4073	049	WAT	X	17	32.659	22.367	51.695	1.00	36.96	8
ATOM	4074	040	WAT	X	18	8.655	11.822	18.551	1.00	22.83	8
ATOM	4075	041	WAT	X	18	61.442	16.332	49.671	1.00	35.09	8
ATOM	4076	042	WAT	X	18	52.691	20.468	49.830	1.00	27.27	8
ATOM	4077	043	WAT	X	18	33.981	29.452	4.620	1.00	46.70	8
ATOM	4078	044	WAT	X	18	22.398	9.094	32.744	1.00	31.90	8
ATOM	4079	045	WAT	X	18	24.654	27.519	4.442	1.00	26.37	8
ATOM	4080	046	WAT	X	18	24.112	52.226	27.595	1.00	38.43	8
ATOM	4081	047	WAT	X	18	33.663	55.271	29.435	1.00	43.20	8
ATOM	4082	048	WAT	X	18	30.748	53.658	50.670	1.00	29.38	8
ATOM	4083	049	WAT	X	18	50.065	24.808	35.502	1.00	35.76	8
ATOM	4084	040	WAT	X	19	22.202	19.032	28.774	1.00	27.27	8
ATOM	4085	041	WAT	X	19	54.614	46.941	48.285	1.00	29.46	8
ATOM	4086	042	WAT	X	19	46.049	21.147	25.366	1.00	33.35	8
ATOM	4087	043	WAT	X	19	45.816	49.038	43.196	1.00	33.55	8
ATOM	4088	044	WAT	X	19	22.659	43.614	47.560	1.00	46.32	8
ATOM	4089	045	WAT	X	19	60.822	30.153	59.870	1.00	43.42	8
ATOM	4090	046	WAT	X	19	53.393	13.840	38.545	1.00	34.26	8
ATOM	4091	047	WAT	X	19	32.544	1.677	6.989	1.00	38.69	8
ATOM	4092	048	WAT	X	19	50.647	31.408	43.808	1.00	33.78	8
ATOM	4093	049	WAT	X	19	16.948	27.505	19.812	1.00	23.95	8
ATOM	4094	040	WAT	X	20	6.330	5.129	-1.860	1.00	35.10	8
ATOM	4095	041	WAT	X	20	32.149	29.484	1.396	1.00	29.24	8
ATOM	4096	042	WAT	X	20	18.952	20.628	24.894	1.00	35.86	8
ATOM	4097	043	WAT	X	20	31.733	56.172	34.803	1.00	38.99	8
ATOM	4098	044	WAT	X	20	54.293	14.452	50.415	1.00	35.67	8
ATOM	4099	045	WAT	X	20	44.169	20.632	26.756	1.00	27.57	8
ATOM	4100	046	WAT	X	20	25.114	53.998	30.655	1.00	43.33	8
ATOM	4101	047	WAT	X	20	43.966	46.309	55.136	1.00	37.54	8
ATOM	4102	048	WAT	X	20	58.366	45.019	48.175	1.00	43.14	8
ATOM	4103	049	WAT	X	20	44.205	21.201	13.125	1.00	51.53	8
ATOM	4104	040	WAT	X	21	61.128	25.016	42.919	1.00	45.95	8
ATOM	4105	041	WAT	X	21	8.371	24.444	12.113	1.00	45.95	8
ATOM	4106	042	WAT	X	21	18.370	31.505	12.739	1.00	27.20	8
ATOM	4107	043	WAT	X	21	33.430	25.045	51.739	1.00	31.92	8
ATOM	4108	044	WAT	X	21	47.660	31.418	59.018	1.00	35.64	8
ATOM	4109	045	WAT	X	21	43.308	25.115	12.609	1.00	40.37	8
ATOM	4110	046	WAT	X	21	44.725	50.787	28.523	1.00	26.83	8
ATOM	4111	047	WAT	X	21	40.073	41.591	56.477	1.00	38.23	8
ATOM	4112	048	WAT	X	21	3.706	15.718	9.641	1.00	23.55	8
ATOM	4113	049	WAT	X	21	46.527	18.879	50.827	1.00	35.55	8
ATOM	4114	040	WAT	X	22	51.052	12.865	45.163	1.00	48.72	8
ATOM	4115	041	WAT	X	22	54.191	42.505	55.913	1.00	22.39	8
ATOM	4116	042	WAT	X	22	65.480	31.263	47.436	1.00	36.62	8
ATOM	4117	043	WAT	X	22	30.283	47.935	54.169	1.00	31.71	8
ATOM	4118	044	WAT	X	22	35.283	36.318	46.899	1.00	68.71	8
ATOM	4119	045	WAT	X	22	47.871	46.056	38.969	1.00	32.78	8
ATOM	4120	046	WAT	X	22	37.896	8.826	3.495	1.00	35.54	8
ATOM	4121	047	WAT	X	22	35.101	8.628	38.130	1.00	35.44	8
ATOM	4122	048	WAT	X	22	38.308	4.945	9.263	1.00	39.44	8
ATOM	4123	049	WAT	X	22	29.192	42.186	18.601	1.00	35.54	8
ATOM	4124	040	WAT	X	23	43.449	25.207	33.605	1.00	42.65	8
ATOM	4125	041	WAT	X	23	42.056	26.583	57.913	1.00	44.04	8
ATOM	4126	042	WAT	X	23	15.436	32.096	27.975	1.00	29.94	8
ATOM	4127	043	WAT	X	23	40.123	43.268	18.152	1.00	37.43	8
ATOM	4128	044	WAT	X	23	14.301	18.529	21.331	1.00	32.32	8
ATOM	4129	045	WAT	X	23	41.316	39.786	58.213	1.00	42.06	8
ATOM	4130	046	WAT	X	23	28.167	15.941	46.987	1.00	39.62	8
ATOM	4131	047	WAT	X	23	62.463	32.861	38.118	1.00	33.05	8
ATOM	4132	048	WAT	X	23	50.420	44.042	41.952	1.00	24.23	8
ATOM	4133	049	WAT	X	23	30.486	6.686	18.716	1.00	37.32	8
ATOM	4134	040	WAT	X	24	39.000	11.315	44.273	1.00	38.40	8

4135	ATOM	04135	041	WAT	X	24	26.342	44.842	18.030	1.00	27.39	8
4136	ATOM	04136	042	WAT	X	24	42.233	42.967	22.516	1.00	28.16	8
4137	ATOM	04137	043	WAT	X	24	17.859	41.857	40.950	1.00	44.87	8
4138	ATOM	04138	044	WAT	X	24	18.774	45.302	36.094	1.00	36.85	8
4139	ATOM	04139	045	WAT	X	24	17.379	48.385	29.218	1.00	34.00	8
4140	ATOM	04140	046	WAT	X	24	59.859	17.628	38.947	1.00	26.40	8
4141	ATOM	04141	047	WAT	X	24	44.716	26.845	15.361	1.00	31.66	8
4142	ATOM	04142	048	WAT	X	24	16.851	22.367	25.144	1.00	38.33	8
4143	ATOM	04143	049	WAT	X	24	44.428	18.344	31.454	1.00	28.87	8
4144	ATOM	04144	040	WAT	X	25	53.824	36.690	57.769	1.00	27.33	8
4145	ATOM	04145	041	WAT	X	25	53.688	40.328	57.339	1.00	34.91	8
4146	ATOM	04146	042	WAT	X	25	46.373	15.118	12.832	1.00	38.80	8
4147	ATOM	04147	043	WAT	X	25	29.609	35.711	7.581	1.00	30.09	8
4148	ATOM	04148	044	WAT	X	25	26.515	13.237	-3.213	1.00	30.52	8
4149	ATOM	04149	045	WAT	X	25	20.273	3.147	6.130	1.00	29.22	8
4150	ATOM	04150	046	WAT	X	25	34.514	42.011	19.633	1.00	23.60	8
4151	ATOM	04151	047	WAT	X	25	41.463	52.238	24.622	1.00	33.83	8
4152	ATOM	04152	048	WAT	X	25	18.346	37.804	42.302	1.00	35.93	8
4153	ATOM	04153	049	WAT	X	25	35.262	54.671	32.179	1.00	58.94	8
4154	ATOM	04154	040	WAT	X	26	44.229	16.673	16.585	1.00	37.25	8
4155	ATOM	04155	041	WAT	X	26	44.766	14.121	14.699	1.00	46.53	8
4156	ATOM	04156	042	WAT	X	26	31.390	33.920	59.134	1.00	33.03	8
4157	ATOM	04157	043	WAT	X	26	12.971	21.397	23.469	1.00	37.99	8
4158	ATOM	04158	044	WAT	X	26	41.259	51.310	51.509	1.00	40.81	8
4159	ATOM	04159	045	WAT	X	26	41.929	11.622	42.697	1.00	45.17	8
4160	ATOM	04160	046	WAT	X	26	42.707	44.751	57.570	1.00	43.32	8
4161	ATOM	04161	047	WAT	X	26	56.463	43.749	51.681	1.00	36.66	8
4162	ATOM	04162	048	WAT	X	26	24.821	11.342	-3.728	1.00	33.27	8
4163	ATOM	04163	049	WAT	X	26	60.493	39.175	53.713	1.00	47.98	8
4164	ATOM	04164	040	WAT	X	27	45.625	38.306	11.910	1.00	37.28	8
4165	ATOM	04165	041	WAT	X	27	43.801	49.874	24.898	1.00	75.50	8
4166	ATOM	04166	042	WAT	X	27	11.684	17.068	21.179	1.00	34.01	8
4167	ATOM	04167	043	WAT	X	27	28.216	2.169	14.807	1.00	42.07	8
4168	ATOM	04168	044	WAT	X	27	52.804	30.867	37.880	1.00	33.10	8
4169	ATOM	04169	045	WAT	X	27	55.458	34.651	38.180	1.00	47.45	8
4170	ATOM	04170	046	WAT	X	27	49.808	19.847	34.189	1.00	33.89	8
4171	ATOM	04171	047	WAT	X	27	1.703	6.632	4.199	1.00	62.88	8
4172	ATOM	04172	048	WAT	X	27	48.275	39.555	43.586	1.00	28.38	8
4173	ATOM	04173	049	WAT	X	27	23.075	20.226	-6.003	1.00	61.62	8
4174	ATOM	04174	040	WAT	X	28	38.679	43.247	57.111	1.00	53.07	8
4175	ATOM	04175	041	WAT	X	28	21.533	51.639	33.545	1.00	49.86	8
4176	ATOM	04176	042	WAT	X	28	1.544	11.851	5.024	1.00	69.29	8
4177	ATOM	04177	043	WAT	X	28	22.566	43.229	15.525	1.00	20.33	8
4178	ATOM	04178	044	WAT	X	28	44.851	57.241	34.859	1.00	42.49	8
4179	ATOM	04179	045	WAT	X	28	33.378	9.541	42.581	1.00	51.22	8
4180	ATOM	04180	046	WAT	X	28	27.186	6.024	-0.021	1.00	46.35	8
4181	ATOM	04181	047	WAT	X	28	56.162	41.254	59.120	1.00	56.59	8
4182	ATOM	04182	048	WAT	X	28	5.756	19.201	7.132	1.00	20.05	8
4183	ATOM	04183	049	WAT	X	28	14.700	29.886	48.605	1.00	35.67	8
4184	ATOM	04184	040	WAT	X	29	41.585	56.275	32.373	1.00	42.13	8
4185	ATOM	04185	041	WAT	X	29	24.086	49.694	43.922	1.00	40.12	8
4186	ATOM	04186	042	WAT	X	29	29.979	22.421	2.045	1.00	42.88	8
4187	ATOM	04187	043	WAT	X	29	18.885	13.752	26.566	1.00	49.31	8
4188	ATOM	04188	044	WAT	X	29	33.246	35.860	58.555	1.00	24.66	8
4189	ATOM	04189	045	WAT	X	29	20.518	10.712	22.033	1.00	31.01	8
4190	ATOM	04190	046	WAT	X	29	28.355	41.870	50.614	1.00	38.09	8
4191	ATOM	04191	047	WAT	X	29	51.144	33.761	38.200	1.00	28.11	8
4192	ATOM	04192	048	WAT	X	29	50.909	32.604	61.158	1.00	44.30	8
4193	ATOM	04193	049	WAT	X	29	45.397	9.987	33.816	1.00	41.23	8
4194	ATOM	04194	040	WAT	X	30	45.383	21.851	32.647	1.00	34.24	8
4195	ATOM	04195	041	WAT	X	30	51.981	22.543	34.910	1.00	43.50	8
4196	ATOM	04196	042	WAT	X	30	35.294	58.821	39.452	1.00	34.28	8
4197	ATOM	04197	043	WAT	X	30	34.193	44.616	18.067	1.00	42.78	8
4198	ATOM	04198	044	WAT	X	30	31.695	52.889	53.190	1.00	56.83	8
4199	ATOM	04199	045	WAT	X	30	13.657	44.210	31.115	1.00	42.94	8
4200	ATOM	04200	046	WAT	X	30	17.493	40.635	13.227	1.00	54.30	8
4201	ATOM	04201	047	WAT	X	30	24.521	11.373	22.566	1.00	42.89	8
4202	ATOM	04202	048	WAT	X	30	37.671	38.607	58.700	1.00	67.82	8
4203	ATOM	04203	049	WAT	X	30	8.539	26.332	10.421	1.00	56.80	8
4204	ATOM	04204	040	WAT	X	31	49.681	16.792	34.456	1.00	56.81	8
4205	ATOM	04205	041	WAT	X	31	7.284	6.777	13.925	1.00	41.62	8
4206	ATOM	04206	042	WAT	X	31	19.842	44.869	37.796	1.00	32.48	8
4207	ATOM	04207	043	WAT	X	31	16.806	43.159	34.050	1.00	31.63	8
4208	ATOM	04208	044	WAT	X	31	40.080	55.247	29.931	1.00	46.41	8
4209	ATOM	04209	045	WAT	X	31	4.298	25.496	15.931	1.00	55.22	8
4210	ATOM	04210	046	WAT	X	31	49.649	40.424	40.847	1.00	31.66	8
4211	ATOM	04211	047	WAT	X	31	22.128	29.127	52.419	1.00	40.80	8
4212	ATOM	04212	048	WAT	X	31	16.243	33.605	36.184	1.00	38.09	8
4213	ATOM	04213	049	WAT	X	31	27.033	55.215	28.323	1.00	31.92	8
4214	ATOM	04214	040	WAT	X	32	16.931	37.637	36.501	1.00	32.22	8
4215	ATOM	04215	041	WAT	X	32	7.050	10.385	16.890	1.00	37.40	8
4216	ATOM	04216	042	WAT	X	32	50.382	29.410	35.312	1.00	56.52	8
4217	ATOM	04217	043	WAT	X	32	27.086	47.626	17.616	1.00	31.50	8
4218	ATOM	04218	044	WAT	X	32	50.029	47.652	42.125	1.00	45.87	8
4219	ATOM	04219	045	WAT	X	32	29.154	55.495	24.292	1.00	53.90	8
4220	ATOM	04220	046	WAT	X	32	32.970	58.606	36.552	1.00	46.22	8
4221	ATOM	04221	047	WAT	X	32	43.201	24.152	56.971	1.00	59.17	8
4222	ATOM	04222	048	WAT	X	32	41.947	30.732	9.284	1.00	45.99	8
4223	ATOM	04223	049	WAT	X	32	21.381	14.261	36.815	1.00	44.69	8
4224	ATOM	04224	040	WAT	X	33	60.941	22.089	43.042	1.00	37.06	8
4225	ATOM	04225	041	WAT	X	33	40.505	56.155	42.947	1.00	68.99	8
4226	ATOM	04226	042	WAT	X	33	18.578	37.434	47.553	1.00	35.06	8
4227	ATOM	04227	043	WAT	X	33	31.707	48.490	18.182	1.00	32.40	8
4228	ATOM	04228	044	WAT	X	33	20.611	21.237	38.626	1.00	41.44	8
4229	ATOM	04229	045	WAT	X	33	38.037	8.708	21.690	1.00	53.54	8
4230	ATOM	04230	046	WAT	X	33	18.925	37.694	11.766	1.00	57.07	8
4231	ATOM	04231	047	WAT	X	33	53.097	28.032	37.987	1.00	57.12	8
4232	ATOM	04232	048	WAT	X	33	63.148	36.349	37.733	1.00	40.38	8
4233	ATOM	04233	049	WAT	X	33	14.116	36.171	21.843	1.00	42.46	8
4234	ATOM	04234	040	WAT	X	34	22.608	32.412	5.553	1.00	37.92	8
4235	ATOM	04235	041	WAT	X	34	29.443	3.779	16.367	1.00	46.74	8
4236	ATOM	04236	042	WAT	X	34	41.862	17.565	7.880	1.00	10.16	8
4237	ATOM	04237	043	WAT	X	34	44.558	18.412	8.333	1.00	38.61	8
4238	ATOM	04238	044	WAT	X	34	51.913	26.058	58.542	1.00	43.05	8
4239	ATOM	04239	045	WAT	X	34	64.063	33.656	56.634	1.00	55.33	8
4240	ATOM	04240	046	WAT	X	34	34.660	53.702	52.276	1.00	47.20	8

ATOM	4241	0428	WAT	X	34	5.844	14.713	12.911	1.00	40.12	8
ATOM	4242	0429	WAT	X	34	39.697	54.257	50.395	1.00	36.68	8
ATOM	4243	0430	WAT	X	35	18.706	24.537	40.234	1.00	51.89	8
ATOM	4244	0431	WAT	X	35	20.209	21.570	34.426	1.00	34.23	8
ATOM	4245	0432	WAT	X	35	44.584	17.646	26.801	1.00	35.48	8
ATOM	4246	0433	WAT	X	35	61.438	32.246	57.799	1.00	36.05	8
ATOM	4247	0434	WAT	X	35	13.266	6.166	0.033	1.00	49.60	8
ATOM	4248	0435	WAT	X	35	42.142	53.175	26.887	1.00	43.15	8
ATOM	4249	0436	WAT	X	35	33.505	54.214	55.522	1.00	56.63	8
ATOM	4250	0437	WAT	X	35	1.397	8.422	6.873	1.00	48.68	8
ATOM	4251	0438	WAT	X	35	47.778	11.907	38.953	1.00	34.48	8
ATOM	4252	0439	WAT	X	35	15.856	27.767	43.603	1.00	55.40	8
ATOM	4253	0440	WAT	X	36	38.734	7.626	16.829	1.00	43.66	8
ATOM	4254	0441	WAT	X	36	10.578	1.628	2.281	1.00	40.52	8
ATOM	4255	0442	WAT	X	36	50.000	33.901	35.051	1.00	49.14	8
ATOM	4256	0443	WAT	X	36	44.622	34.879	33.356	1.00	60.84	8
ATOM	4257	0444	WAT	X	36	3.016	16.327	21.555	1.00	60.04	8
ATOM	4258	0445	WAT	X	36	41.431	56.503	45.767	1.00	53.09	8
ATOM	4259	0446	WAT	X	36	49.548	26.337	22.216	1.00	53.09	8
ATOM	4260	0447	WAT	X	36	37.549	29.346	4.956	1.00	52.92	8
ATOM	4261	0448	WAT	X	36	53.734	18.532	52.401	1.00	51.95	8
ATOM	4262	0449	WAT	X	36	39.043	11.166	25.898	1.00	36.59	8
ATOM	4263	0450	WAT	X	37	10.532	4.916	16.271	1.00	58.74	8
ATOM	4264	0451	WAT	X	37	41.346	7.373	32.768	1.00	47.04	8
ATOM	4265	0452	WAT	X	37	32.476	41.914	15.484	1.00	44.27	8
ATOM	4266	0453	WAT	X	37	18.592	28.534	17.648	1.00	41.36	8
ATOM	4267	0454	WAT	X	37	58.677	25.814	40.128	1.00	40.22	8
ATOM	4268	0455	WAT	X	37	15.547	6.537	19.083	1.00	45.33	8
ATOM	4269	0456	WAT	X	37	37.675	57.053	47.412	1.00	49.88	8
ATOM	4270	0457	WAT	X	37	49.434	37.594	42.185	1.00	39.96	8
ATOM	4271	0458	WAT	X	37	42.690	28.862	30.545	1.00	42.38	8
ATOM	4272	0459	WAT	X	37	29.822	6.331	24.708	1.00	48.41	8
ATOM	4273	0460	WAT	X	38	16.119	10.852	3.221	1.00	36.08	8
ATOM	4274	0461	WAT	X	38	66.051	14.381	33.005	1.00	54.04	8
ATOM	4275	0462	WAT	X	38	26.231	44.941	50.291	1.00	58.57	8
ATOM	4276	0463	WAT	X	38	51.550	26.375	9.990	1.00	50.76	8
ATOM	4277	0464	WAT	X	38	38.215	7.892	41.087	1.00	49.03	8
ATOM	4278	0465	WAT	X	38	49.722	41.667	12.969	1.00	47.74	8
ATOM	4279	0466	WAT	X	39	35.909	18.255	51.330	1.00	59.07	8
ATOM	4280	0467	WAT	X	39	43.924	10.373	31.316	1.00	53.37	8
ATOM	4281	0468	WAT	X	39	22.583	10.397	39.495	1.00	42.79	8
ATOM	4282	0469	WAT	X	39	19.514	68.906	21.847	1.00	68.43	8
ATOM	4283	0470	WAT	X	39	13.468	27.723	5.713	1.00	66.89	8
ATOM	4284	0471	WAT	X	39	45.654	25.542	63.943	1.00	44.03	8
ATOM	4285	0472	WAT	X	39	44.078	13.029	36.066	1.00	37.57	8
ATOM	4286	0473	WAT	X	39	27.240	0.087	12.290	1.00	48.13	8
ATOM	4287	0474	WAT	X	39	15.804	17.374	23.289	1.00	45.09	8
ATOM	4288	0475	WAT	X	40	23.294	12.036	34.534	1.00	58.48	8
ATOM	4289	0476	WAT	X	40	47.490	44.003	18.065	1.00	60.75	8
ATOM	4290	0477	WAT	X	40						
ATOM	4291	0478	WAT	X	40						
ATOM	4292	0479	WAT	X	40						
ATOM	4293	0480	WAT	X	40						
ATOM	4294	0481	WAT	X	40						
ATOM	4295	0482	WAT	X	40						
ATOM	4296	0483	WAT	X	40						
ATOM	4297	0484	WAT	X	40						
ATOM	4298	0485	WAT	X	40						
ATOM	4299	0486	WAT	X	40						
ATOM	4300	0487	WAT	X	40						
ATOM	4301	0488	WAT	X	40						
ATOM	4302	0489	WAT	X	40						
ATOM	4303	0490	WAT	X	40						
ATOM	4304	0491	WAT	X	40						
ATOM	4305	0492	WAT	X	40						
ATOM	4306	0493	WAT	X	40						
ATOM	4307	0494	WAT	X	40						
ATOM	4308	0495	WAT	X	40						
ATOM	4309	0496	WAT	X	40						
ATOM	4310	0497	WAT	X	40						
ATOM	4311	0498	WAT	X	40						
ATOM	4312	0499	WAT	X	40						
ATOM	4313	0500	WAT	X	40						
ATOM	4314	0501	WAT	X	40						
ATOM	4315	0502	WAT	X	40						
ATOM	4316	0503	WAT	X	40						
ATOM	4317	0504	WAT	X	40						
ATOM	4318	0505	WAT	X	40						
ATOM	4319	0506	WAT	X	40						
ATOM	4320	0507	WAT	X	40						
ATOM	4321	0508	WAT	X	40						
ATOM	4322	0509	WAT	X	40						
ATOM	4323	0510	WAT	X	40						
ATOM	4324	0511	WAT	X	40						
ATOM	4325	0512	WAT	X	40						
ATOM	4326	0513	WAT	X	40						
ATOM	4327	0514	WAT	X	40						
ATOM	4328	0515	WAT	X	40						
ATOM	4329	0516	WAT	X	40						
ATOM	4330	0517	WAT	X	40						
ATOM	4331	0518	WAT	X	40						
ATOM	4332	0519	WAT	X	40						
ATOM	4333	0520	WAT	X	40						
ATOM	4334	0521	WAT	X	40						
ATOM	4335	0522	WAT	X	40						
ATOM	4336	0523	WAT	X	40						
ATOM	4337	0524	WAT	X	40						
ATOM	4338	0525	WAT	X	40						
ATOM	4339	0526	WAT	X	40						
ATOM	4340	0527	WAT	X	40						
ATOM	4341	0528	WAT	X	40						
ATOM	4342	0529	WAT	X	40						
ATOM	4343	0530	WAT	X	40						
ATOM	4344	0531	WAT	X	40						
ATOM	4345	0532	WAT	X	40						
ATOM	4346	0533	WAT	X	40						

4347	ATOM	0405	WAT	X	45	15.297	36.178	30.314	1.00	41.94	8
4348	ATOM	0406	WAT	X	45	11.948	34.622	19.560	1.00	83.16	8
4349	ATOM	0408	WAT	X	45	49.746	24.887	60.391	1.00	66.28	8
4350	ATOM	0409	WAT	X	45	36.657	55.115	28.131	1.00	37.69	8
4351	ATOM	0405	WAT	X	46	55.074	25.248	36.950	1.00	41.36	8
4352	ATOM	0401	WAT	X	46	47.652	23.423	22.484	1.00	42.59	8
4353	ATOM	0402	WAT	X	46	44.015	15.772	24.447	1.00	47.57	8
4354	ATOM	0403	WAT	X	46	7.635	2.279	10.856	1.00	61.51	8
4355	ATOM	0404	WAT	X	46	55.490	45.238	53.756	1.00	80.18	8
4356	ATOM	0405	WAT	X	46	24.651	30.369	3.824	1.00	53.51	8
4357	ATOM	0406	WAT	X	46	36.564	25.795	58.795	1.00	53.24	8
4358	ATOM	0407	WAT	X	46	37.878	24.510	56.673	1.00	60.23	8
4359	ATOM	0408	WAT	X	46	9.767	27.253	17.228	1.00	44.01	8
4360	ATOM	0409	WAT	X	46	33.066	7.229	37.529	1.00	48.47	8
4361	ATOM	0401	WAT	X	47	8.243	21.706	21.929	1.00	61.56	8
4362	ATOM	0402	WAT	X	47	46.978	13.274	45.175	1.00	40.90	8
4363	ATOM	0403	WAT	X	47	41.004	12.753	21.561	1.00	73.88	8
4364	ATOM	0404	WAT	X	47	3.035	8.918	-0.355	1.00	50.88	8
4365	ATOM	0405	WAT	X	47	18.537	34.248	10.555	1.00	79.91	8
4366	ATOM	0406	WAT	X	47	26.233	6.791	-2.079	1.00	48.58	8
4367	ATOM	0407	WAT	X	47	37.312	53.735	22.566	1.00	63.31	8
4368	ATOM	0408	WAT	X	47	17.940	29.638	6.277	1.00	57.32	8
4369	ATOM	0409	WAT	X	47	28.830	27.316	2.717	1.00	62.15	8
4370	ATOM	0401	WAT	X	48	65.931	-28.577	46.176	1.00	69.51	8
4371	ATOM	0402	WAT	X	48	19.661	45.120	40.540	1.00	40.74	8
4372	ATOM	0403	WAT	X	48	10.667	22.744	23.628	1.00	36.22	8
4373	ATOM	0404	WAT	X	48	8.702	24.434	20.838	1.00	51.66	8
4374	ATOM	0405	WAT	X	48	35.773	26.533	56.343	1.00	38.96	8
4375	ATOM	0406	WAT	X	48	38.218	2.333	13.072	1.00	37.60	8
4376	ATOM	0407	WAT	X	48	25.061	48.128	50.748	1.00	69.43	8
4377	ATOM	0408	WAT	X	48	24.333	37.538	52.402	1.00	33.69	8
4378	ATOM	0409	WAT	X	48	52.741	13.029	46.552	1.00	46.94	8
4379	ATOM	0401	WAT	X	49	30.393	18.085	52.715	1.00	73.77	8
4380	ATOM	0402	WAT	X	49	21.293	35.987	52.496	1.00	56.71	8
4381	ATOM	0403	WAT	X	49	26.704	53.743	20.826	1.00	82.73	8
4382	ATOM	0404	WAT	X	49	65.451	38.921	50.670	1.00	50.91	8
4383	ATOM	0405	WAT	X	49	9.019	18.103	21.967	1.00	57.54	8
4384	ATOM	0406	WAT	X	49	43.689	31.759	26.580	1.00	33.20	8
4385	ATOM	0407	WAT	X	49	65.973	31.154	38.950	1.00	51.21	8
4386	ATOM	0408	WAT	X	49	50.668	41.968	57.102	1.00	65.20	8
4387	ATOM	0409	WAT	X	49	67.466	32.818	48.733	1.00	35.55	8
4388	ATOM	0401	WAT	X	50	12.540	31.451	14.136	1.00	67.07	8
4389	ATOM	0402	WAT	X	50	24.089	6.493	18.874	1.00	41.89	8
4390	ATOM	0403	WAT	X	50	46.352	12.360	48.271	1.00	78.91	8
4391	ATOM	0404	WAT	X	50	26.960	36.851	6.038	1.00	44.57	8
4392	ATOM	0405	WAT	X	50	37.082	59.754	36.774	1.00	64.16	8
4393	ATOM	0406	WAT	X	50	57.220	36.380	35.486	1.00	60.08	8
4394	ATOM	0407	WAT	X	50	47.460	48.140	35.950	1.00	51.89	8
4395	ATOM	0408	WAT	X	50	32.642	7.671	29.026	1.00	67.07	8
4396	ATOM	0409	WAT	X	50	40.898	5.278	12.690	1.00	58.45	8
4397	ATOM	0401	WAT	X	51	43.951	11.795	23.808	1.00	51.02	8
4398	ATOM	0402	WAT	X	51	56.331	38.665	59.400	1.00	77.23	8
4399	ATOM	0403	WAT	X	51	42.112	15.859	19.271	1.00	42.44	8
4400	ATOM	0404	WAT	X	51	43.751	9.508	10.207	1.00	72.09	8
4401	ATOM	0405	WAT	X	51	21.156	18.175	-5.366	1.00	59.15	8
4402	ATOM	0406	WAT	X	51	20.822	20.591	30.625	1.00	53.15	8
4403	ATOM	0407	WAT	X	51	25.847	41.728	50.223	1.00	53.16	8
4404	ATOM	0408	WAT	X	51	42.406	49.560	54.444	1.00	49.42	8
4405	ATOM	0409	WAT	X	51	11.152	-0.096	4.529	1.00	73.12	8
4406	ATOM	0401	WAT	X	52	41.064	10.519	39.198	1.00	76.33	8
4407	ATOM	0402	WAT	X	52	11.838	45.652	26.174	1.00	52.20	8
4408	ATOM	0403	WAT	X	52	24.803	8.502	38.134	1.00	48.46	8
4409	ATOM	0404	WAT	X	52	28.241	55.029	32.933	1.00	56.81	8
4410	ATOM	0405	WAT	X	52	24.326	46.042	48.362	1.00	42.89	8
4411	ATOM	0406	WAT	X	52	60.372	23.243	57.581	1.00	51.66	8
4412	ATOM	0407	WAT	X	52	44.063	13.149	3.195	1.00	73.23	8
4413	ATOM	0408	WAT	X	52	29.959	38.273	7.993	1.00	74.96	8
4414	ATOM	0409	WAT	X	52	35.761	36.887	7.808	1.00	46.76	8
4415	ATOM	0401	WAT	X	53	29.185	14.140	50.554	1.00	100.00	8
4416	ATOM	0402	WAT	X	53	46.852	47.409	54.235	1.00	47.47	8
4417	ATOM	0403	WAT	X	53	46.126	18.871	10.000	1.00	74.45	8
4418	ATOM	0404	WAT	X	53	43.467	42.127	14.225	1.00	58.70	8
4419	ATOM	0405	WAT	X	53	42.354	10.824	26.570	1.00	74.16	8
4420	ATOM	0406	WAT	X	53	41.382	9.160	28.416	1.00	65.06	8
4421	ATOM	0407	WAT	X	53	32.249	16.276	51.085	1.00	66.53	8
4422	ATOM	0408	WAT	X	53	43.754	20.935	55.297	1.00	89.21	8
4423	ATOM	0409	WAT	X	53	46.525	22.435	61.833	1.00	64.40	8
4424	ATOM	0401	WAT	X	54	36.489	9.501	46.403	1.00	43.78	8
4425	ATOM	0402	WAT	X	54	13.785	14.234	21.394	1.00	46.49	8
4426	ATOM	0403	WAT	X	54	44.108	8.308	6.121	1.00	74.38	8
4427	ATOM	0404	WAT	X	54	37.095	13.297	47.553	1.00	92.89	8
4428	ATOM	0405	WAT	X	54	60.222	38.361	56.675	1.00	71.18	8
4429	ATOM	0406	WAT	X	54	43.676	52.104	52.067	1.00	52.01	8
4430	ATOM	0407	WAT	X	54	13.472	23.519	26.526	1.00	85.06	8
4431	ATOM	0408	WAT	X	54	26.573	48.774	55.241	1.00	63.24	8
4432	ATOM	0409	WAT	X	54	38.373	54.655	25.877	1.00	61.51	8
4433	ATOM	0401	WAT	X	55	40.109	29.004	7.323	1.00	50.80	8
4434	ATOM	0402	WAT	X	55	40.897	28.228	33.474	1.00	55.10	8
4435	ATOM	0403	WAT	X	55	26.359	57.407	32.671	1.00	74.31	8
4436	ATOM	0404	WAT	X	55	15.383	36.694	13.336	1.00	63.36	8
4437	ATOM	0405	WAT	X	55	25.637	23.526	51.791	1.00	62.36	8
4438	ATOM	0406	WAT	X	55	47.868	37.197	21.724	1.00	98.01	8
4439	ATOM	0407	WAT	X	55	48.664	28.592	20.875	1.00	61.42	8
4440	ATOM	0408	WAT	X	55	22.182	11.543	42.550	1.00	50.93	8
4441	ATOM	0409	WAT	X	55	14.290	33.767	23.519	1.00	43.45	8
4442	ATOM	0401	WAT	X	56	49.254	21.261	57.388	1.00	74.77	8
4443	ATOM	0402	WAT	X	56	32.072	50.437	56.442	1.00	84.60	8
4444	ATOM	0403	WAT	X	56	6.861	26.478	7.012	1.00	69.24	8
4445	ATOM	0404	WAT	X	56	36.069	6.771	2.277	1.00	89.64	8
4446	ATOM	0405	WAT	X	56	60.239	29.387	37.677	1.00	64.46	8
4447	ATOM	0406	WAT	X	56	46.693	15.300	46.504	1.00	37.40	8
4448	ATOM	0407	WAT	X	56	47.685	47.802	26.981	1.00	44.40	8
4449	ATOM	0408	WAT	X	56	21.472	47.007	15.910	1.00	70.01	8
4450	ATOM	0409	WAT	X	56	2.967	21.682	5.603	1.00	60.74	8
4451	ATOM	0401	WAT	X	57	62.723	25.567	58.195	1.00	45.51	8
4452	ATOM	0402	WAT	X	57						8

ATOM	4453	046	WAT	X	56	53.874	20.460	35.843	1.00	60.27	0
ATOM	4454	047	WAT	X	56	34.043	6.968	31.691	1.00	54.01	0
ATOM	4455	048	WAT	X	56	20.830	41.835	12.224	1.00	100.00	0
ATOM	4456	049	WAT	X	56	16.599	30.946	13.916	1.00	37.38	0
ATOM	4457	040	WAT	X	57	44.358	21.696	26.084	1.00	64.44	0
ATOM	4458	041	WAT	X	57	9.788	63.318	30.716	1.00	90.76	0
ATOM	4459	042	WAT	X	57	65.207	28.476	57.189	1.00	72.19	0
ATOM	4460	043	WAT	X	57	20.871	4.547	-1.268	1.00	64.52	0
ATOM	4461	045	WAT	X	57	24.856	36.282	6.866	1.00	55.25	0
ATOM	4462	047	WAT	X	57	65.931	24.875	58.247	1.00	42.06	0
ATOM	4463	048	WAT	X	57	41.604	10.565	45.137	1.00	80.93	0
ATOM	4464	049	WAT	X	57	30.736	44.603	54.453	1.00	58.39	0
ATOM	4465	040	WAT	X	58	22.167	48.706	40.870	1.00	52.19	0
ATOM	4466	041	WAT	X	58	66.082	25.557	51.546	1.00	48.90	0
ATOM	4467	043	WAT	X	58	25.692	34.825	52.948	1.00	50.59	0
ATOM	4468	045	WAT	X	58	26.160	51.696	48.736	1.00	44.75	0
ATOM	4469	046	WAT	X	58	56.334	43.153	40.380	1.00	53.34	0
ATOM	4470	045	WAT	X	58	30.990	17.627	55.917	1.00	84.28	0
ATOM	4471	046	WAT	X	58	45.287	39.941	7.939	1.00	57.03	0
ATOM	4472	047	WAT	X	58	3.405	18.650	9.230	1.00	73.95	0
ATOM	4473	048	WAT	X	58	54.294	19.752	55.578	1.00	50.99	0
ATOM	4474	049	WAT	X	58	44.732	52.287	54.381	1.00	75.96	0
ATOM	4475	040	WAT	X	59	47.776	51.035	36.798	1.00	53.81	0
ATOM	4476	041	WAT	X	59	29.391	47.450	56.869	1.00	86.62	0
ATOM	4477	042	WAT	X	59	38.808	50.946	52.782	1.00	47.24	0
ATOM	4478	043	WAT	X	59	20.090	10.595	-7.477	1.00	69.34	0
ATOM	4479	044	WAT	X	59	30.700	10.315	45.674	1.00	63.75	0
ATOM	4480	045	WAT	X	59	60.018	46.795	44.900	1.00	57.35	0
ATOM	4481	046	WAT	X	59	46.214	52.834	49.312	1.00	67.99	0
ATOM	4482	047	WAT	X	59	56.880	28.891	60.457	1.00	85.53	0
ATOM	4483	048	WAT	X	59	36.201	48.379	58.178	1.00	71.18	0
ATOM	4484	049	WAT	X	59	35.313	2.318	16.129	1.00	66.51	0
ATOM	4485	040	WAT	X	60	34.944	58.828	34.422	1.00	69.27	0
ATOM	4486	041	WAT	X	60	47.891	40.270	60.882	1.00	62.61	0
ATOM	4487	042	WAT	X	60	20.100	54.046	30.414	1.00	91.37	0
ATOM	4488	043	WAT	X	60	0.688	22.084	15.126	1.00	65.51	0
ATOM	4489	044	WAT	X	60	50.911	50.933	54.227	1.00	45.99	0
ATOM	4490	045	WAT	X	60	50.514	44.428	38.574	1.00	67.41	0
ATOM	4491	046	WAT	X	60	31.208	54.171	26.648	1.00	65.99	0
ATOM	4492	047	WAT	X	60	49.541	38.319	60.498	1.00	49.78	0
ATOM	4493	048	WAT	X	60	23.270	55.339	31.653	1.00	66.17	0
ATOM	4494	049	WAT	X	60	46.551	15.109	50.163	1.00	87.28	0
ATOM	4495	040	WAT	X	61	65.999	24.860	47.686	1.00	57.42	0
ATOM	4496	041	WAT	X	61	30.573	36.197	57.967	1.00	51.73	0
ATOM	4497	042	WAT	X	61	3.779	13.380	-2.503	1.00	65.73	0
ATOM	4498	043	WAT	X	61	48.944	12.221	41.061	1.00	39.29	0
ATOM	4499	045	WAT	X	61	66.745	25.656	43.289	1.00	52.05	0
ATOM	4500	046	WAT	X	61	51.657	40.026	13.448	1.00	48.71	0
ATOM	4501	047	WAT	X	61	27.718	47.942	52.615	1.00	34.81	0
ATOM	4502	048	WAT	X	61	24.460	41.243	12.842	1.00	65.85	0
ATOM	4503	049	WAT	X	61	2.848	14.406	12.411	1.00	61.94	0
ATOM	4504	040	WAT	X	62	23.747	48.989	47.991	1.00	55.02	0
ATOM	4505	041	WAT	X	62	63.167	23.291	45.841	1.00	64.42	0
ATOM	4506	042	WAT	X	62	55.731	29.439	38.673	1.00	64.37	0
ATOM	4507	043	WAT	X	62	39.039	4.879	14.767	1.00	52.29	0
ATOM	4508	044	WAT	X	62	43.782	27.030	47.614	1.00	5.00	0
ATOM	4509	045	WAT	X	62	27.765	34.219	1.860	1.00	67.67	0
ATOM	4510	046	WAT	X	62	65.774	20.800	46.451	1.00	72.56	0
ATOM	4511	047	WAT	X	62	65.823	27.727	48.583	1.00	52.36	0
ATOM	4512	048	WAT	X	63	47.510	11.024	43.713	1.00	70.64	0
ATOM	4513	049	WAT	X	63	66.150	30.203	50.411	1.00	51.22	0
ATOM	4514	040	WAT	X	63	48.089	20.346	31.711	1.00	85.43	0
ATOM	4515	041	WAT	X	63	16.744	26.725	47.695	1.00	81.36	0
ATOM	4516	042	WAT	X	63	19.203	31.730	8.203	1.00	67.60	0
ATOM	4517	043	WAT	X	63	18.178	51.891	26.673	1.00	68.28	0
ATOM	4518	044	WAT	X	63	31.035	55.837	30.147	1.00	80.95	0
ATOM	4519	045	WAT	X	63	34.256	54.728	25.341	1.00	59.54	0
ATOM	4520	046	WAT	X	63	44.621	47.771	25.528	1.00	61.68	0
ATOM	4521	047	WAT	X	63	16.999	27.936	51.121	1.00	52.06	0
ATOM	4522	048	WAT	X	63	36.358	38.943	11.274	1.00	69.59	0
ATOM	4523	049	WAT	X	63	16.484	22.381	39.229	1.00	36.64	0
ATOM	4524	040	WAT	X	64	23.799	46.745	46.122	1.00	62.10	0
ATOM	4525	041	WAT	X	64	30.457	7.355	-1.129	1.00	72.94	0
ATOM	4526	042	WAT	X	64	19.222	33.502	3.190	1.00	50.09	0
ATOM	4527	043	WAT	X	64	46.509	18.371	25.238	1.00	62.10	0
ATOM	4528	044	WAT	X	64	32.283	10.295	-4.119	1.00	76.54	0
ATOM	4529	045	WAT	X	64	11.959	41.211	33.089	1.00	65.37	0
ATOM	4530	046	WAT	X	64	19.983	24.672	46.573	1.00	75.52	0
ATOM	4531	047	WAT	X	64	9.603	26.690	3.912	1.00	76.73	0
ATOM	4532	048	WAT	X	64	45.825	9.757	40.836	1.00	67.39	0
ATOM	4533	049	WAT	X	64	49.404	34.287	20.920	1.00	83.61	0
ATOM	4534	040	WAT	X	64	21.346	51.355	35.980	1.00	69.62	0
ATOM	4535	041	WAT	X	64	34.793	9.610	-4.714	1.00	63.30	0
ATOM	4536	042	WAT	X	64	6.006	27.070	13.534	1.00	58.69	0
ATOM	4537	043	WAT	X	64	57.091	33.822	60.700	1.00	69.62	0
ATOM	4538	044	WAT	X	64	11.853	27.880	7.921	1.00	63.30	0
ATOM	4539	045	WAT	X	64	35.486	56.715	40.693	1.00	57.61	0
ATOM	4540	046	WAT	X	64	20.467	20.497	41.249	1.00	69.67	0
ATOM	4541	047	WAT	X	64	37.508	57.667	34.228	1.00	55.12	0
ATOM	4542	048	WAT	X	64	8.621	27.294	14.167	1.00	67.33	0
ATOM	4543	049	WAT	X	64	3.733	19.033	3.659	1.00	66.26	0
ATOM	4544	040	WAT	X	64	18.954	18.854	32.541	1.00	61.60	0
ATOM	4545	041	WAT	X	64	25.346	2.504	1.837	1.00	67.71	0
ATOM	4546	042	WAT	X	64	34.927	1.355	1.837	1.00	65.35	0
ATOM	4547	043	WAT	X	64	47.719	47.565	30.106	1.00	61.68	0
ATOM	4548	044	WAT	X	64	58.933	17.613	53.979	1.00	71.56	0
ATOM	4549	045	WAT	X	64	16.418	40.606	47.124	1.00	65.35	0
ATOM	4550	046	WAT	X	64	33.051	35.235	6.368	1.00	63.11	0
ATOM	4551	047	WAT	X	64	10.404	2.233	-1.826	1.00	71.56	0
ATOM	4552	048	WAT	X	64	27.844	10.427	43.773	1.00	65.38	0
ATOM	4553	049	WAT	X	64	9.821	19.794	23.580	1.00	74.16	0
ATOM	4554	040	WAT	X	64	34.906	24.545	27.529	1.00	77.66	0
ATOM	4555	041	WAT	X	64	42.873	50.245	43.593	1.00	82.51	0
ATOM	4556	042	WAT	X	64	11.780	40.835	20.822	1.00	57.23	0
ATOM	4557	043	WAT	X	64	23.833	50.272	22.080	1.00	57.23	0

4559	ATOM	0459	043	WAT	X	70	12.149	0.500	-0.175	1.00100.00	8
4560	ATOM	0460	044	WAT	X	70	24.781	48.147	16.489	1.00 53.74	8
4561	ATOM	0461	045	WAT	X	70	45.295	18.629	15.166	1.00 66.52	8
4562	ATOM	0462	046	WAT	X	70	16.273	24.172	43.929	1.00 86.28	8
4563	ATOM	0463	047	WAT	X	71	14.692	0.299	4.588	1.00 76.24	8
4564	ATOM	0464	048	WAT	X	71	56.655	15.988	46.443	1.00 74.53	8
4565	ATOM	0465	049	WAT	X	71	44.653	15.572	21.500	1.00 81.92	8
4566	ATOM	0466	050	WAT	X	71	13.915	34.012	32.549	1.00 76.95	8
4567	ATOM	0467	051	WAT	X	72	18.894	23.324	28.037	1.00 69.01	8
4568	ATOM	0468	052	WAT	X	72	25.942	27.526	52.380	1.00 80.30	8
4569	ATOM	0469	053	WAT	X	72	20.444	43.760	44.743	1.00 57.92	8
4570	ATOM	0470	054	WAT	X	72	56.463	15.927	56.362	1.00 90.66	8
4571	ATOM	0471	055	WAT	X	72	67.258	38.530	40.380	1.00 67.91	8
4572	ATOM	0472	056	WAT	X	73	13.119	23.916	-2.569	1.00 57.58	8
4573	ATOM	0473	057	WAT	X	73	27.753	4.319	2.523	1.00 68.14	8
4574	ATOM	0474	058	WAT	X	73	15.049	27.612	26.066	1.00 71.85	8
4575	ATOM	0475	059	WAT	X	73	41.506	30.331	28.071	1.00 39.96	8
4576	ATOM	0476	060	WAT	X	73	49.356	13.175	50.180	1.00 77.21	8
4577	ATOM	0477	061	WAT	X	74	44.776	9.064	36.247	1.00 56.22	8
4578	ATOM	0478	062	WAT	X	74	14.995	33.147	12.393	1.00 74.77	8
4579	ATOM	0479	063	WAT	X	74	21.394	18.327	43.796	1.00 77.10	8
4580	ATOM	0480	064	WAT	X	74	-0.275	3.244	2.071	1.00 89.93	8
4581	ATOM	0481	065	WAT	X	74	32.705	3.566	1.290	1.00100.00	8
4582	ATOM	0482	066	WAT	X	74	32.871	44.907	16.023	1.00 71.10	8
4583	ATOM	0483	067	WAT	X	74	41.289	9.005	3.932	1.00 71.97	8
4584	ATOM	0484	068	WAT	X	75	39.329	57.673	44.241	1.00 64.90	8
4585	ATOM	0485	069	WAT	X	75	18.910	30.958	52.593	1.00 93.30	8
4586	ATOM	0486	070	WAT	X	75	68.020	36.610	50.288	1.00 86.49	8
4587	ATOM	0487	071	WAT	X	76	22.139	39.199	7.275	1.00 71.53	8
4588	ATOM	0488	072	WAT	X	76	58.720	42.672	38.660	1.00 68.73	8
4589	ATOM	0489	073	WAT	X	76	61.482	44.540	47.192	1.00 77.48	8
4590	ATOM	0490	074	WAT	X	76	22.107	41.072	47.776	1.00 60.73	8
4591	ATOM	0491	075	WAT	X	77	2.634	-1.318	3.949	1.00 69.96	8
4592	ATOM	0492	076	WAT	X	77	32.187	5.643	25.223	1.00 76.13	8
4593	ATOM	0493	077	WAT	X	77	67.602	33.066	51.363	1.00 72.23	8
4594	ATOM	0494	078	WAT	X	77	52.748	50.627	48.547	1.00 74.39	8
4595	ATOM	0495	079	WAT	X	77	10.204	44.509	25.769	1.00 64.94	8
4596	ATOM	0496	080	WAT	X	77	22.754	10.234	24.846	1.00 66.60	8
4597	ATOM	0497	081	WAT	X	78	65.372	34.387	54.026	1.00 68.26	8
4598	ATOM	0498	082	WAT	X	78	61.952	23.010	40.260	1.00 64.44	8
4599	ATOM	0499	083	WAT	X	78	6.141	-0.725	6.920	1.00 63.43	8
4600	ATOM	0500	084	WAT	X	78	62.946	40.127	37.159	1.00 74.61	8
4601	ATOM	0501	085	WAT	X	79	57.524	45.787	43.333	1.00 68.47	8
4602	ATOM	0502	086	WAT	X	79	27.601	6.844	22.540	1.00100.00	8
4603	ATOM	0503	087	WAT	X	79	13.772	31.115	20.743	1.00 37.33	8
4604	ATOM	0504	088	WAT	X	79	58.663	23.880	36.310	1.00 71.62	8
4605	ATOM	0505	089	WAT	X	79	49.511	45.784	34.237	1.00 64.41	8
4606	ATOM	0506	090	WAT	X	80	42.349	10.479	16.376	1.00 86.89	8
4607	ATOM	0507	091	WAT	X	80	64.430	36.390	57.479	1.00 81.60	8
4608	ATOM	0508	092	WAT	X	80	51.348	32.222	6.850	1.00 86.83	8
4609	ATOM	0509	093	WAT	X	80	28.165	8.846	38.088	1.00 71.08	8
4610	ATOM	0510	094	WAT	X	81	65.757	27.493	53.760	1.00 48.10	8
4611	ATOM	0511	095	WAT	X	81	45.249	12.674	37.874	1.00 50.64	8
4612	ATOM	0512	096	WAT	X	81	13.341	34.872	38.349	1.00 64.64	8
4613	ATOM	0513	097	WAT	X	81	51.626	42.754	59.455	1.00 87.45	8
4614	ATOM	0514	098	WAT	X	81	17.748	40.786	43.576	1.00 81.62	8
4615	ATOM	0515	099	WAT	X	81	40.981	31.297	32.687	1.00 92.90	8
4616	ATOM	0516	100	WAT	X	81	36.339	42.304	57.906	1.00 54.44	8
4617	ATOM	0517	001	WAT	X	82	52.150	44.557	55.997	1.00 81.29	8
4618	ATOM	0518	002	WAT	X	82	44.696	27.699	29.800	1.00 66.84	8
4619	ATOM	0519	003	WAT	X	82	15.369	42.073	36.641	1.00 87.69	8
4620	ATOM	0520	004	WAT	X	82	44.262	38.613	61.725	1.00 74.79	8
4621	ATOM	0521	005	WAT	X	82	10.887	37.555	22.160	1.00 77.71	8
4622	ATOM	0522	006	WAT	X	82	57.317	26.895	38.482	1.00 54.04	8
4623	ATOM	0523	007	WAT	X	83	1.485	10.546	14.639	1.00 49.60	8
4624	ATOM	0524	008	WAT	X	83	44.383	11.585	44.954	1.00 69.75	8
4625	ATOM	0525	009	WAT	X	83	13.091	19.080	23.540	1.00 84.10	8
4626	ATOM	0526	010	WAT	X	83	49.664	18.609	50.424	1.00 79.36	8
4627	ATOM	0527	011	WAT	X	83	-0.411	-0.186	6.219	1.00 73.91	8
4628	ATOM	0528	012	WAT	X	84	-0.060	12.467	10.762	1.00 74.36	8
4629	ATOM	0529	013	WAT	X	84	45.916	18.172	53.625	1.00 82.88	8
4630	ATOM	0530	014	WAT	X	84	42.886	23.516	61.123	1.00 71.70	8
4631	ATOM	0531	015	WAT	X	84	26.711	5.741	19.232	1.00 65.61	8
4632	ATOM	0532	016	WAT	X	84	18.341	21.188	47.071	1.00 79.82	8
4633	ATOM	0533	017	WAT	X	84	30.324	37.264	55.283	1.00 63.21	8
4634	ATOM	0534	018	WAT	X	84	45.383	21.545	29.439	1.00 65.08	8
4635	ATOM	0535	019	WAT	X	85	47.617	21.423	28.329	1.00 72.90	8
4636	ATOM	0536	020	WAT	X	85	14.724	8.133	-4.054	1.00 80.41	8
4637	ATOM	0537	021	WAT	X	85	10.404	38.900	34.440	1.00 73.60	8
4638	ATOM	0538	022	WAT	X	85	30.311	39.411	56.032	1.00 72.07	8
4639	ATOM	0539	023	WAT	X	86	38.750	51.931	56.443	1.00 83.88	8
4640	ATOM	0540	024	WAT	X	86	28.737	50.755	56.620	1.00 78.91	8
4641	ATOM	0541	025	WAT	X	86	38.447	9.203	1.111	1.00 60.02	8
4642	ATOM	0542	026	WAT	X	86	63.955	18.750	55.290	1.00 75.30	8
4643	ATOM	0543	027	WAT	X	86	28.437	41.435	56.329	1.00 77.99	8
4644	ATOM	0544	028	WAT	X	86	27.951	49.707	19.814	1.00 80.66	8
4645	ATOM	0545	029	WAT	X	86	33.978	8.299	40.249	1.00 69.22	8
4646	ATOM	0546	030	WAT	X	86	17.498	1.498	10.616	1.00 71.37	8
4647	ATOM	0547	031	WAT	X	87	1.278	15.798	6.438	1.00 70.87	8
4648	ATOM	0548	032	WAT	X	87	37.174	55.569	52.513	1.00 69.91	8
4649	ATOM	0549	033	WAT	X	87	68.146	21.047	55.397	1.00 70.79	8
4650	ATOM	0550	034	WAT	X	87	24.655	52.548	24.459	1.00 72.31	8
4651	ATOM	0551	035	WAT	X	87	46.009	24.086	33.287	1.00 79.02	8
4652	ATOM	0552	036	WAT	X	87	50.195	14.529	36.835	1.00 65.15	8
4653	ATOM	0553	037	WAT	X	88	29.201	3.240	-2.272	1.00 78.74	8
4654	ATOM	0554	038	WAT	X	88	13.357	32.036	24.857	1.00 62.05	8
4655	ATOM	0555	039	WAT	X	88	65.406	20.886	50.995	1.00 76.49	8
4656	ATOM	0556	040	WAT	X	88	20.515	8.228	19.759	1.00 73.98	8
4657	ATOM	0557	041	WAT	X	88	46.758	18.587	30.455	1.00 74.75	8
4658	ATOM	0558	042	WAT	X	89	49.679	43.124	20.824	1.00 80.84	8
4659	ATOM	0559	043	WAT	X	89	60.303	44.435	40.737	1.00 70.62	8
4660	ATOM	0560	044	WAT	X	89	13.240	-1.159	9.184	1.00 78.53	8
4661	ATOM	0561	045	WAT	X	89	61.700	19.538	53.061	1.00 64.93	8
4662	ATOM	0562	046	WAT	X	89	24.291	28.301	0.472	1.00 69.68	8
4663	ATOM	0563	047	WAT	X	90	27.964	24.098	-2.600	1.00 84.61	8
4664	ATOM	0564	048	WAT	X	90	22.140	24.413	52.912	1.00 67.47	8

4665	ATOM	QW3	WAT	X	90	39.112	6.740	5.054	1.00	66.72	8
4666	ATOM	QW4	WAT	X	90	43.364	57.890	49.964	1.00	71.30	8
4667	ATOM	QW6	WAT	X	90	16.187	27.842	27.844	1.00	71.63	8
4668	ATOM	QW7	WAT	X	90	22.913	3.223	6.101	1.00	63.36	8
4669	ATOM	QW0	WAT	X	91	0.373	23.417	18.644	1.00	68.95	8
4670	ATOM	QW1	WAT	X	91	19.144	22.297	52.147	1.00	68.45	8
4671	ATOM	QW2	WAT	X	91	46.750	22.374	17.228	1.00	68.56	8
4672	ATOM	QW3	WAT	X	91	50.310	39.246	9.155	1.00	68.48	8
4673	ATOM	QW5	WAT	X	91	14.832	31.811	-1.674	1.00	65.32	8
4674	ATOM	QW6	WAT	X	91	39.568	22.971	59.682	1.00	94.75	8
4675	ATOM	QW0	WAT	X	92	28.305	37.474	53.688	1.00	64.82	8
4676	ATOM	QW1	WAT	X	92	60.842	35.037	35.557	1.00	68.20	8
4677	ATOM	QW3	WAT	X	92	38.306	2.043	9.940	1.00	74.71	8
4678	ATOM	QW4	WAT	X	92	37.932	10.010	23.873	1.00	62.54	8
4679	ATOM	QW5	WAT	X	92	37.872	59.284	31.560	1.00	64.40	8
4680	ATOM	QW8	WAT	X	92	16.587	37.900	45.458	1.00	57.48	8
4681	ATOM	QW2	WAT	X	93	24.426	6.991	31.450	1.00	62.04	8
4682	ATOM	QW3	WAT	X	93	15.322	46.823	24.885	1.00	68.48	8
4683	ATOM	QW5	WAT	X	93	18.754	23.194	42.946	1.00	49.72	8
4684	ATOM	QW6	WAT	X	93	20.917	46.805	43.439	1.00	45.25	8
4685	ATOM	QW8	WAT	X	93	28.767	42.761	53.085	1.00	51.35	8
4686	ATOM	QW0	WAT	X	94	32.517	16.473	33.381	1.00	60.16	8
4687	ATOM	QW2	WAT	X	94	26.635	4.800	29.351	1.00	63.33	8
4688	ATOM	QW3	WAT	X	94	1.194	4.216	9.172	1.00	60.36	8
4689	ATOM	QW4	WAT	X	94	25.652	19.885	-5.299	1.00	58.09	8
4690	ATOM	QW5	WAT	X	94	43.661	12.692	20.184	1.00	65.23	8
4691	ATOM	QW6	WAT	X	94	17.439	46.586	41.518	1.00	66.21	8
4692	ATOM	QW7	WAT	X	94	35.133	15.487	30.639	1.00	49.75	8
4693	ATOM	QW8	WAT	X	94	36.346	8.698	18.844	1.00	48.58	8
4694	ATOM	QW0	WAT	X	95	30.818	8.165	40.636	1.00	56.86	8
4695	ATOM	QW1	WAT	X	95	40.089	21.776	55.765	1.00	53.69	8
4696	ATOM	QW2	WAT	X	95	18.639	14.065	-5.612	1.00	55.94	8
4697	ATOM	QW3	WAT	X	95	51.587	38.457	41.331	1.00	56.04	8
4698	ATOM	QW4	WAT	X	95	50.107	29.401	17.255	1.00	56.00	8
4699	ATOM	QW5	WAT	X	95	8.218	14.744	20.596	1.00	56.95	8
4700	ATOM	QW6	WAT	X	95	40.674	47.760	57.927	1.00	54.91	8

CLAIMS

1. A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least
5 one altered property as compared to said parent α -amylase, which method comprises

i) analysing the structure of the parent Termamyl-like α -amylase to identify at least one amino acid residue or at least
10 one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is believed to be of relevance for altering said property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations),

15

ii) constructing a Termamyl-like α -amylase variant, which as compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

20

iii) testing the resulting Termamyl-like α -amylase variant for said property.

2. The method according to claim 1, wherein the property to be
25 altered is selected from the group consisting of substrate specificity, substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6) or high (e.g. pH>9) pH values), stability towards oxidation, Ca^{2+} -
30 dependency and specific activity.

3. The method according to claim 1 or 2, wherein the property to be altered is the calcium ion dependency and the structural part to be modified is selected from the group consisting of
35 the C domain, the interface between the A and B domain, the interface between the A and C domain, or the interaction to a calcium binding site of the Termamyl-like α -amylase.

4. The method according to claim 1 or 2, wherein the property to be altered is the substrate cleavage pattern and the structural part to be modified is located within 10Å from an amino acid residue of the substrate binding site.

5

5. A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method comprises

- 10 i) comparing the three-dimensional structure of the Termamyl-like α -amylase with the structure of a non-Termamyl-like α -amylase,
- ii) identifying a part of the Termamyl-like α -amylase structure which is different from the non-Termamyl-like α -amylase
15 structure and which from structural or functional considerations is contemplated to be responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α -amylase, and
- iii) modifying the part of the Termamyl-like α -amylase
20 identified in ii) whereby a Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α -amylase.

6. The method according to claim 6, wherein, in step iii), the
25 part of the Termamyl-like α -amylase is modified so as to resemble the corresponding part of the non-Termamyl-like α -amylase.

7. The method according to claim 5 or 6, wherein, in step iii),
30 the modification is accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified; by replacing one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified with the amino acid residues occupying corresponding positions in the
35 non-Termamyl-like α -amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α -amylase into a corresponding position in the Termamyl-like α -amylase.

8. The method according to any of claims 5-7, wherein the non-Termamyl-like α -amylase structure is the structure of a fungal α -amylase or a mammalian α -amylase.
- 5 9. The method according to claim 8, wherein the non-Termamyl-like α -amylase is the *Aspergillus oryzae* TAKA α -amylase, the *A. niger* acid α -amylase, the *Bacillus subtilis* α -amylase or the pig pancreatic α -amylase.
- 10 10. The method according to any of claims 1-9, wherein the parent Termamyl-like α -amylase is derived from a strain of *Bacillus*.
11. The method according to claim 10, wherein the parent α -
15 amylase is derived from a strain of a *B. licheniformis*, *B. amyloliquefaciens*, *B. stearothermophilus* or a strain from an alkalophilic *Bacillus* sp. such as NCIB 12289, NCIB 12512 or NCIB 12513.
- 20 12. The method according to any of claims 1-11, wherein the parent α -amylase is a hybrid α -amylase comprising a combination of partial amino acid sequences derived from at least two α -amylases, of which one is a Termamyl-like α -amylase and the other(s) are, e.g., from a microbial and/or a mammalian α -
25 amylase.
13. The method according to any of claims 5-12, wherein the part of the parent Termamyl-like α -amylase to be modified and identified in step ii) is loop 1, loop 2, loop 3 and/or loop 8
30 of the parent α -amylase.
13. A method of constructing a variant of a parent Termamyl-like α -amylase, which has a decreased calcium ion dependency as compared to said parent, which method comprises:
- 35 i) identifying an amino acid residue within 10Å from a Ca²⁺ binding site of a Termamyl-like α -amylase in a model of the three-dimensional structure of said α -amylase, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,

- ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural
5 or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and
iii) testing the Ca^{2+} dependency of the resulting Termamyl-like α -amylase variant.

- 10 14. A method of constructing a variant of a parent Termamyl-like α -amylase which variant has α -amylase activity and an altered pH dependent activity, which method comprises

i) in a three-dimensional structure of the Termamyl-like α -
15 amylase in question, identifying an amino acid residue within 15\AA from an active site residue, in particular 10\AA from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue,

20

ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and evaluating the accomodation of the amino acid residue in the
25 structure,

iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into the structure,

30

iv) constructing a Termamyl-like α -amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent activity of said variant.

- 35 15. A method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α -amylase, which method comprises

- i) identifying an internal hole or a crevice of the parent Termamyl-like α -amylase in the three-dimensional structure of said α -amylase,
- ii) replacing, in the structure, one or more amino acid
5 residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of the hole or crevice,
- 10 iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.

16. A method of constructing a variant of a Termamyl-like α -
15 amylase which has a reduced ability to cleave a substrate close to the branching point, which method comprises

- i) identifying the substrate binding area of the parent Termamyl-like α -amylase in a model of the three-dimensional
20 structure of said α -amylase,
- ii) replacing, in the model, one or more amino acid residues of the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of
25 the parent α -amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding
30 one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and
- iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the substrate cleavage pattern of the
35 variant.

17. The method according to any of the preceeding claims, in which the α -amylase variant is obtained by cultivating a

microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth.

5

18. A variant of a parent Termamyl-like α -amylase, in which variant at least one amino acid residue of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ
10 ID No. 4, has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of
15 SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

19. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of
20 variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No
25 10, wherein

X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,

30 Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and

V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

35 20. The variant according to claim 18 or 19, wherein X is the amino acid residue occupying position 48 and Y the amino acid residue occupying position 51 of SEQ ID NO 4 and Z is the amino

acid residue occupying position 70 and V the amino acid residue occupying position 78 in SEQ ID No 10.

21. A variant of a parent Termamyl-like α -amylase, in which
5 variant at least one of the amino acid residues of the parent
 α -amylase, which is/are present in an amino acid fragment
corresponding to the amino acid fragment 195-202 of the amino
acid sequence of SEQ ID No. 4, has been deleted or replaced
with one or more of the amino acid residues which is/are
10 present in an amino acid fragment corresponding to the amino
acid fragment 165-177 of the amino acid sequence shown in SEQ
ID No. 10, or in which one or more additional amino acid
residues has been added using the relevant part of SEQ ID No.
10 or a corresponding part of another Fungamyl-like α -amylase
15 as a template.

22. A variant of a parent Termamyl-like α -amylase, which
variant has a region which, when the amino acid sequence of
variant is aligned most closely with the amino acid sequence of
20 the said parent α -amylase, occupies the same position as the
portion from residue X to residue Y of SEQ ID No 4, the said
region having at least 80%, such as 90% sequence homology with
the part of SEQ ID No 10 extending from residue Z to residue V
of SEQ ID No 10, wherein
25 X is the amino acid occupying position 195 or 196 of SEQ ID No.
4,

Y is the amino acid residue occupying position 198, 199, 200,
201, or 202 of SEQ ID No. 4,

30

Z is the amino acid residue occupying position 165 or 166 of
SEQ ID No. 10, and

V is the amino acid residue occupying position 173, 174, 175,
35 176 or 177 of SEQ ID No. 10.

23. The variant according to claim 21 or 22, in which the amino
acid fragment of the parent α -amylase, which corresponds to

amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

5

24. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of
10 SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added
15 using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

25. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of
20 variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue
25 Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

30 Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

35

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

26. The variant according to claim 24 or 25, in which an amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

27. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

20

28. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

29. The variant according to claim 27 or 28, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

10

30. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

31. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

Y is the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

35 Z is the amino acid occupying position 28, 29, 30, 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

32. The variant according to claim 30 or 31, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

33. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

34. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein X is the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,

Z is the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

35

V is the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

35. The variant according to claim 33 or 34, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

36. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

37. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 2, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

Y is the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

38. The variant according to claim 36 or 37, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

39. A variant of a parent Fungamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α -amylase as a template.

20

40. A variant of a parent Fungamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 10, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 4, wherein X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 10,

30

Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

35 Z is the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

41. The variant according to claim 39 or 40, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

10

42. A variant according to any of claims 39-41, in which the the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 4.

43. A variant of a parent Fungamyl-like α -amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the amino acid sequence shown in SEQ ID No. 10 has been deleted.

45. A variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a decreased Ca^{2+} dependency as compared to the parent α -amylase.

46. A variant according to claim 45, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID NO 2:

30 N104, A349, I479, L346, I430, N457, K385, F350, I411, H408 or G303, in particular a mutation corresponding to

N104D;

A349C+I479C;

L346C+I430C;

35 N457D,E;

N457D,E+K385R;

F350D,E+I430R,K;

F350D,E+I411R,K;

H408Q,E,N,D; and/or
G303N,D,Q,E.

47. A variant of a parent Termamyl-like α -amylase which
5 exhibits a higher activity below the pH optimum than the parent
 α -amylase, which variant comprises a mutation of an amino acid
residue corresponding to at least one of the following
positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):
E336, Q333, P331, I236, V102, A232, I103, L196, in particular
10 at least one of the following mutations:

E336R,K;
Q333R,K; P331R,K;
V102R,K,A,T,S,G;
I236K,R,N;
15 I103K,R;
L196K,R; and/or
A232T,S,G.

48. A variant of a parent Termamyl-like α -amylase which
20 exhibits a higher activity above the pH optimum than the parent
 α -amylase, which variant comprises a mutation of an amino acid
residue corresponding to at least one of the following
positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):
N236, H281 and/or Y273, in particular one of the following
25 mutations:

N326I,Y,F,L,V;
H281F,I,L; and/or
Y273F,W.

30 49. A variant of a parent Termamyl-like α -amylase which
exhibits α -amylase activity and which has an increased
thermostability and/or altered temperature optimum as compared
to the parent α -amylase, which variant comprises a mutation of
an amino acid residue corresponding to at least one of the
35 following positions of the *B. licheniformis* α -amylase (SEQ ID
NO 2):

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143, R146, L241, I236, L7, V259, F284, F350, F343, L427 and/or V481, in particular at least one of the following mutations:

L61W,V,F;

5 Y62W;

F67W;

K106R,F,W;

G145F,W

I212F,L,W,Y,R,K;

10 S151 replaced with any other amino acid residue and in particular with F,W,I or L;

R214W;

Y150R,K;

F143W;

15 R146W;

L241I,F,Y,W;

I236L,F,W,Y;

L7F,I,W;

V259F,I,L;

20 F284W;

F350W;

F343W;

L427F,L,W; and/or

V481,F,I,L,W.

25

50. A variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a reduced capability of cleaving an oligo-saccharide substrate close to the branching point as compared to the parent α -amylase, which
30 variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

V54, D53, Y56, Q333 and/or G57, in particular at least one of
35 the following mutations:

V54L,I,F,Y,W,R,K,H,E,Q;

D53L,I,F,Y,W;

Y,56W;

Q333W; and/or

G57 to all possible amino acid residues.

51. The variant according to any of claims 17-50, wherein one
s or more proline residues present in the amino acid residues
with which the parent α -amylase is modified are replaced with
a non-proline residue such as alanine.

52. The variant according to any of claims 17-51, wherein one
10 or more cysteine residues present in the amino acid residues
with which the parent α -amylase is modified are replaced with
a non-cysteine residue such as alanine.

53. A DNA construct comprising a DNA sequence encoding an α -
15 amylase variant according to any of claims 17-52.

54. A recombinant expression vector which carries a DNA con-
struct according to Claim 53.

20 55. A cell which is transformed with a DNA construct according
to Claim 53 or a vector according to Claim 54.

56. A cell according to Claim 55, which is a microorganism.

25 57. A cell according to Claim 56, which is a bacterium or a
fungus.

58. The cell according to Claim 57, which is a grampositive
bacterium such as *Bacillus subtilis*, *Bacillus licheniformis*,
30 *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*,
Bacillus alkalophilus, *Bacillus amyloliquefaciens*, *Bacillus*
coagulans, *Bacillus circulans*, *Bacillus lautus* or *Bacillus thu-*
ringiensis.

35 59. Use of an α -amylase variant according to any of claims 17-
52 for washing and/or dishwashing.

60. Use of an α -amylase variant according to any of claims 17-52 for desizing.

61. Use of an α -amylase variant according to any of claims 17-52 for starch liquefaction.

62. A detergent additive comprising an α -amylase variant according to any of claims 17-52, optionally in the form of a non-dusting granulate, stabilised liquid or protected enzyme.

10

63. A detergent additive according to Claim 62 which contains 0.02-200 mg of enzyme protein/g of the additive.

64. A detergent additive according to Claim 62 or 63, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

65. A detergent composition comprising an α -amylase variant according to any of claims 17-52.

66. A detergent composition according to Claim 65 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

25

67. A manual or automatic dishwashing detergent composition comprising an α -amylase variant according to any of claims 17-52.

68. A dishwashing detergent composition according to Claim 67 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

69. A manual or automatic laundry washing composition comprising an α -amylase variant according to any of claims 17-52.

70. A laundry washing composition according to Claim 69, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, an amylolytic enzyme and/or a cellulase.

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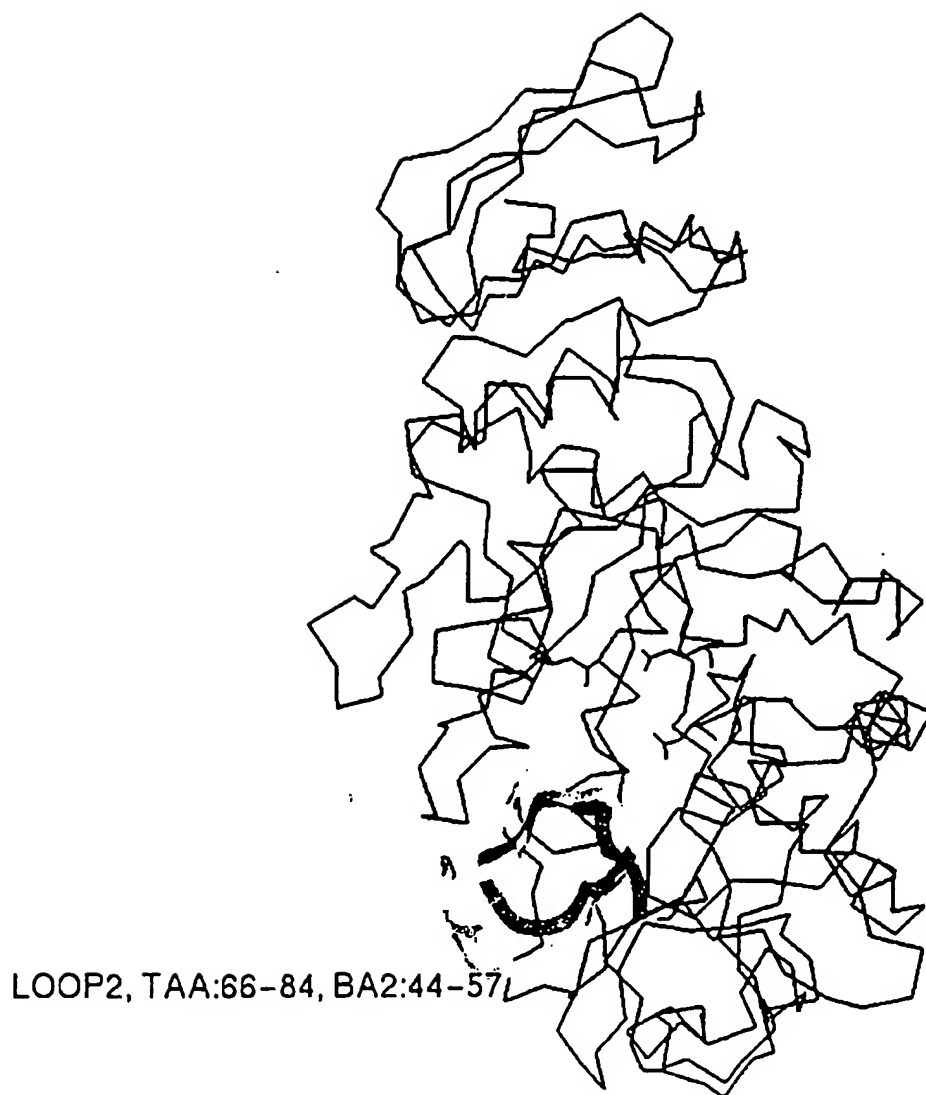
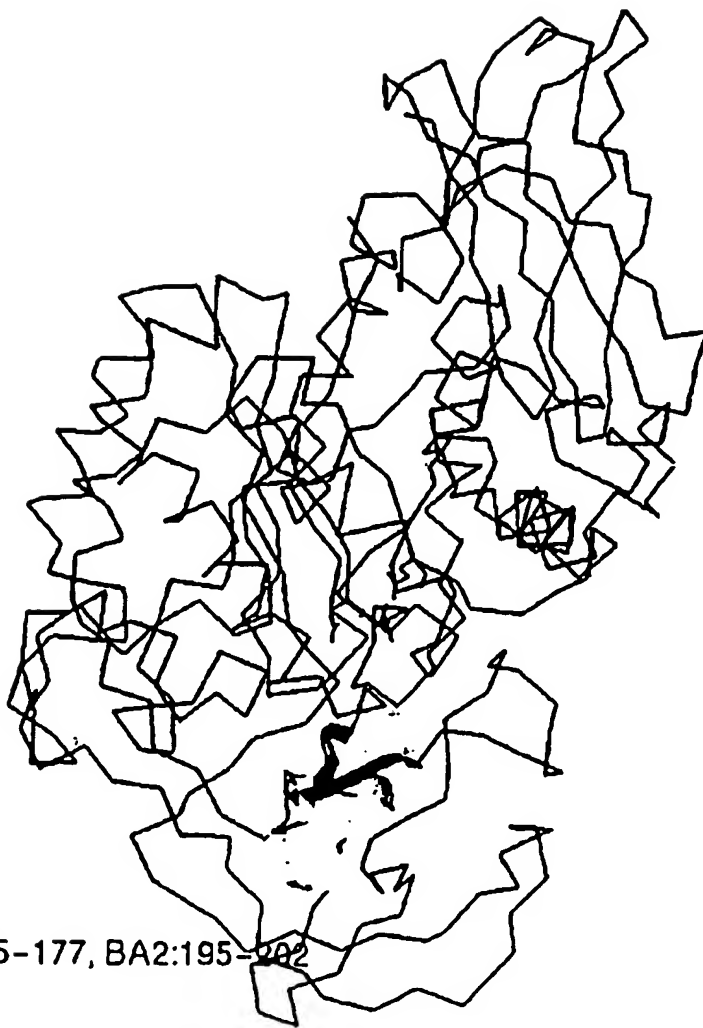


Fig. 1

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LOOP3 (a), TAA:165-177, BA2:195-202

Fig. 2

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Fig. 3

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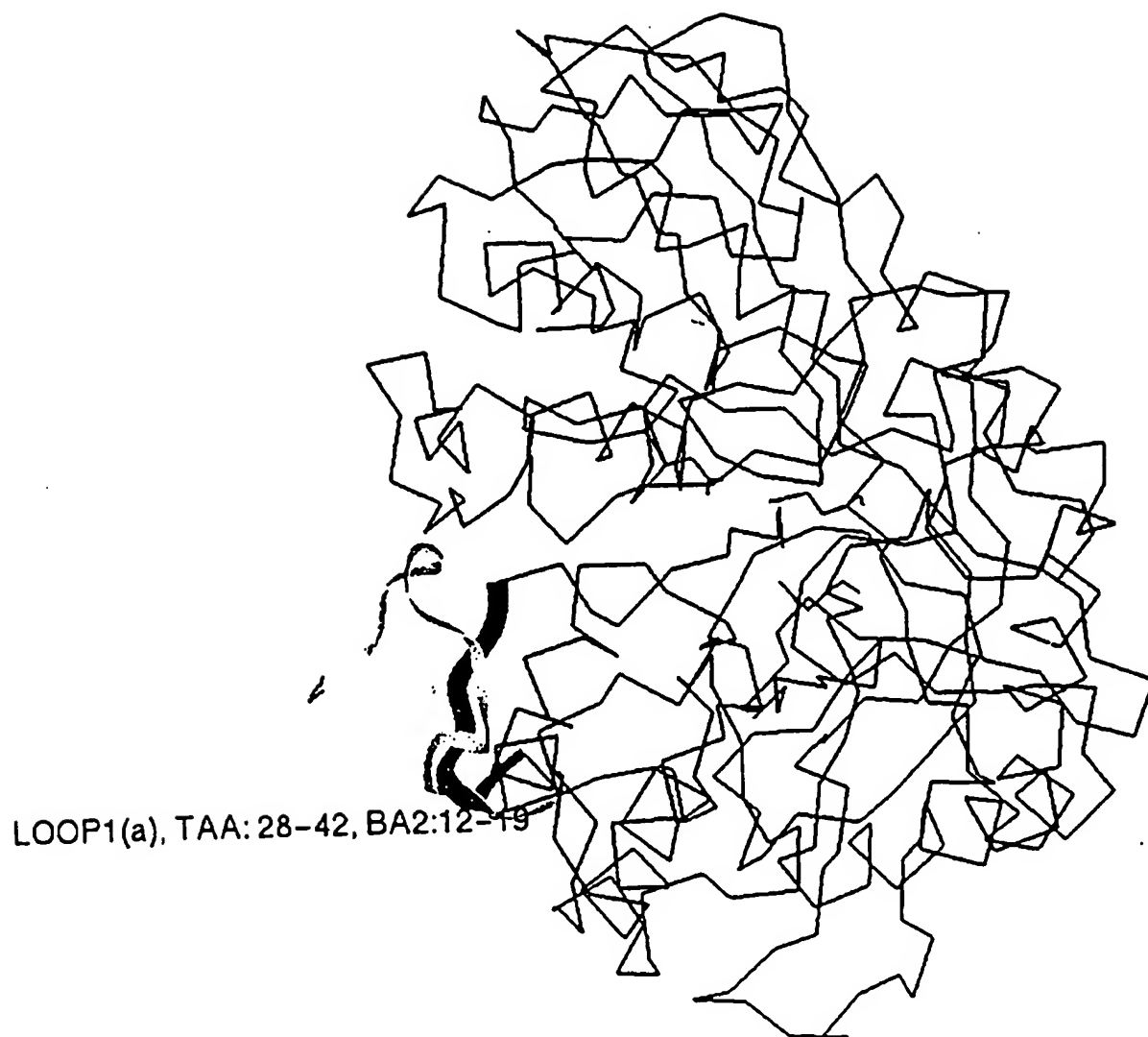


Fig. 4

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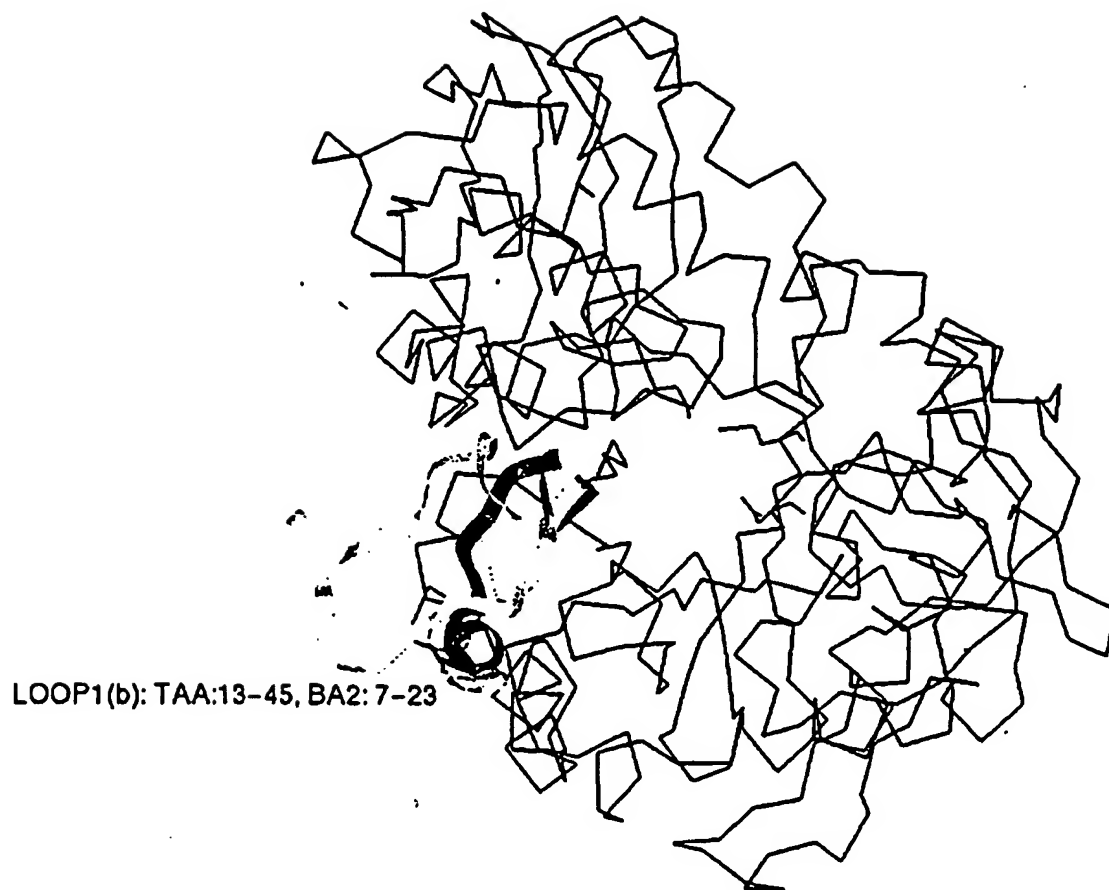


Fig. 5

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LOOP8:TAA:291-313, BA2: 322-346

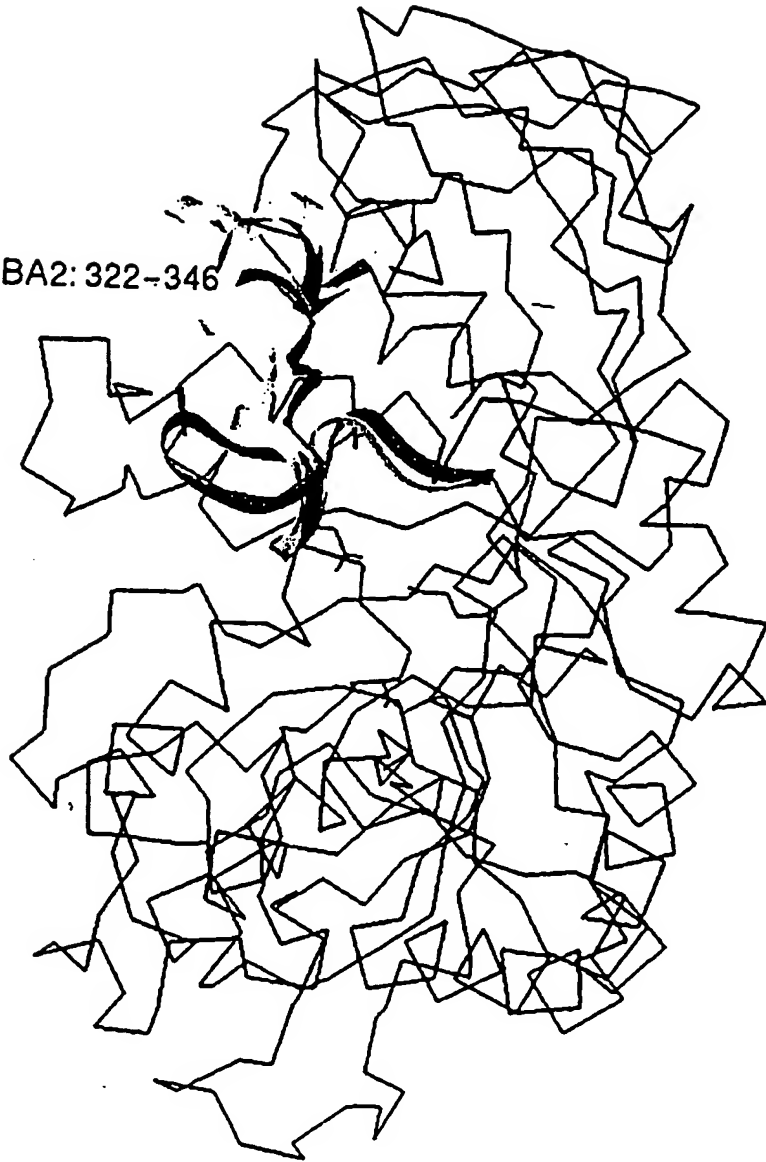


Fig. 6

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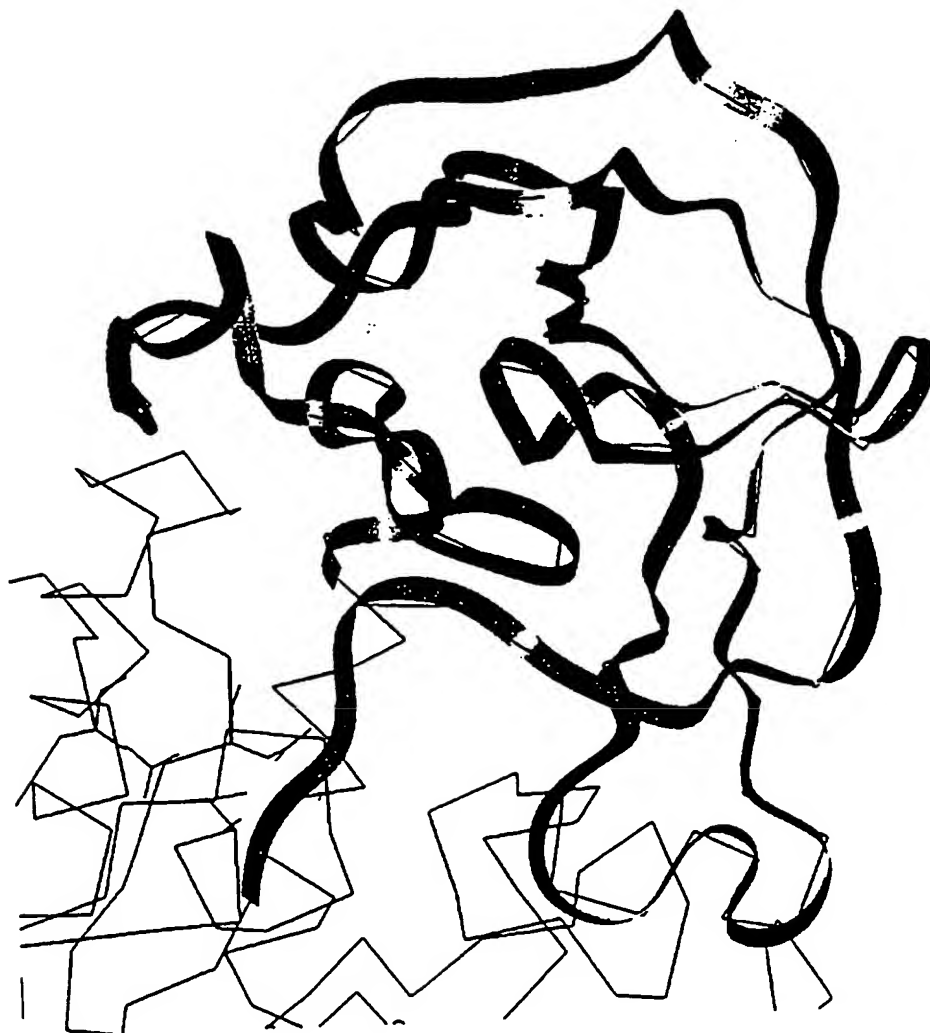


Fig. 7

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1
CAT CAT AAT GGA ACA AAT GGT ACT ATG ATG CAA TAT TTC GAA TGG TAT TTG CCA AAT GAC
H H N G T N G T M M Q Y F E W Y L P N D

21
GGG AAT CAT TGG AAC AGG TTG AGG GAT GAC GCA GCT AAC TTA AAG AGT AAA GGG ATA ACA
G N H W N R L R D D A A N L K S K G I T

41
GCT GTA TGG ATC CCA CCT GCA TGG AAG GGG ACT TCC CAG AAT GAT GTA GGT TAT GGA GCC
A V W I P P A W K G T S Q N D V G Y G A

61
TAT GAT TTA TAT GAT CTT GGA GAG TTT AAC CAG AAG GGG ACG GTT CGT ACA AAA TAT GGA
Y D L Y D L G E F N Q K G T V R T K Y G

81
ACA CGC AAC CAG CTA CAG GCT CGC GTG ACC TCT TTA AAA AAT AAC GGC ATT CAG GTA TAT
T R N Q L Q A A V T S L K N N G I Q V Y

101
GGT GAT GTC GTC ATG AAT CAT AAA GGT GGA GCA GAT GGT ACG GAA ATT GTA AAT GCG GTA
G D V V M N H K G G A D G T E I V N A V

121
GAA GTG AAT CGG AGC AAC CGA AAC CAG GAA ACC TCA GGA GAG TAT GCA ATA GAA GCG TGG
E V N R S N R N Q E T S G E Y A I E A W

141
ACA AAG TTT GAT TTT CCT GGA AGA GGA AAT AAC CAT TCC AGC TTT AAG TGG CGC TGG TAT
T K F D F P G R G N N H S S F K W R W Y

161
CAT TTT GAT GGG ACA GAT TGG GAT CAG TCA CGC CAG CTT CAA AAC AAA ATA TAT AAA TTC
H F D G T D W D Q S R Q L Q N K I Y X F

181
AGG GGA ACA GGC AAG GCC TGG GAC TGG GAA GTC GAT ACA GAG AAT GGC AAC TAT GAC TAT
R G T G K A W D W E V D T E N G N Y D Y

201
CTT ATG TAT GCA GAC GTG GAT ATG GAT CAC CCA GAA GTA ATA CAT GAA CTT AGA AAC TGG
L M Y A D V D M D H P E V I H E L R N W

221
GGA GTG TGG TAT ACG AAT ACA CTG AAC CTT GAT GGA TTT AGA ATA GAT GCA GTG AAA CAT
G V W Y T N T L N L D G F R I D A V K H

241
ATA AAA TAT AGC TTT ACG AGA GAT TGG CTT ACA CAT GTG CGT AAC ACC ACA GGT AAA CCA
I K Y S F T R D W L T H V R N T T G K P

261
ATG TTT GCA GTG GCT GAG TTT TGG AAA AAT GAC CTT GGT GCA ATT GAA AAC TAT TTG AAT
M F A V A E F W K N D L G A I E N Y L N

281
AAA ACA AGT TGG AAT CAC TCG GTG TTT GAT GTT CCT CTC CAC TAT AAT TTG TAC AAT GCA
K T S W N H S V F D V P L H Y N L Y N A

Fig. 8

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301

TCT AAT AGC GGT GGT TAT TAT GAT ATG AGA AAT ATT TTA AAT GGT TCT GTG GTG CAA AAA
S N S G G Y Y D M R N I L N G S V V Q K

321

CAT CCA ACA CAT GCC GTT ACT TTT GTT GAT AAC CAT GAT TCT CAG CCC GGG GAA GCA TTG
H P T H A V T F V D N H D S Q P G E A L

341

GAA TCC TTT GTT CAA CAA TGG TTT AAA CCA CTT GCA TAT GCA TTG GTT CTG ACA AGG GAA
E S F V Q Q W F K P L A Y A L V L T R E

361

CAA GGT TAT CCT TCC GTA TTT TAT GGG GAT TAC TAC GGT ATC CCA ACC CAT GGT GTT CCG
Q G Y P S V F Y G D Y Y G I P T H G V P

381

GCT ATG AAA TCT AAA ATA GAC CCT CTT CTG CAG GCA CGT CAA ACT TTT GCC TAT GGT ACG
A M K S K I D P L L Q A R Q T F A Y G T

401

CAG CAT GAT TAC TTT GAT CAT CAT GAT ATT ATC GGT TGG ACA AGA GAG GGA AAT AGC TCC
Q H D Y F D H H D I I G W T R E G N S S

421

CAT CCA AAT TCA GGC CTT GCC ACC ATT ATG TCA GAT GGT CCA GGT GGT AAC AAA TGG ATG
H P N S G L A T I M S D G P G G N X W M

441

TAT GTG GGG AAA AAT AAA GCG GGA CAA GTT TGG AGA GAT ATT ACC GGA AAT AGG ACA GGC
Y V G K N K A G Q V W R D I T G N R T G

261

ACC GTC ACA ATT AAT GCA GAC GGA TGG GGT AAT TTC TCT GTT AAT GGA GGG TCC GTT TCG
T V T I N A D G W G N F S V N G G S V S

481

GTT TGG GTG AAG CAA TAA
V W V K Q

Fig. 8 (cont.)

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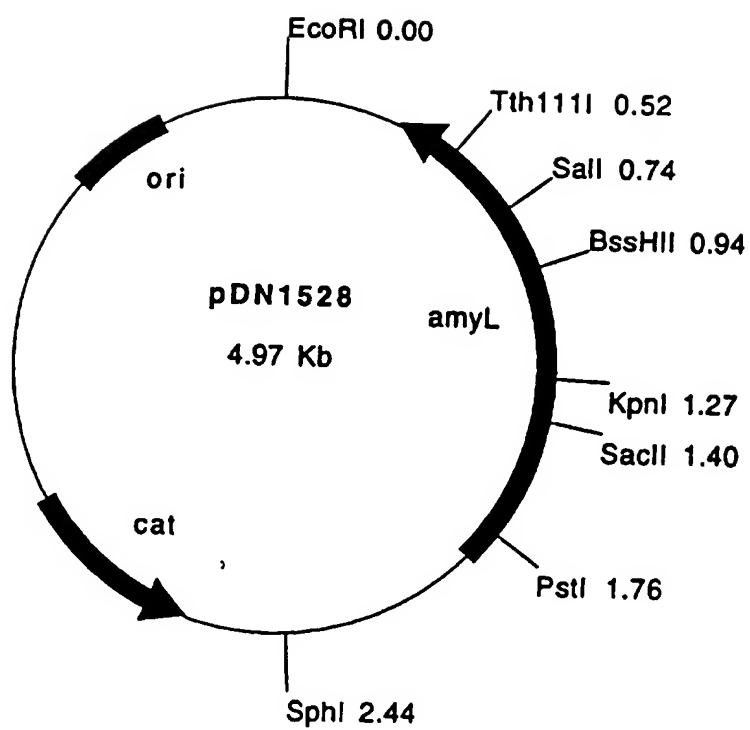


Fig. 9

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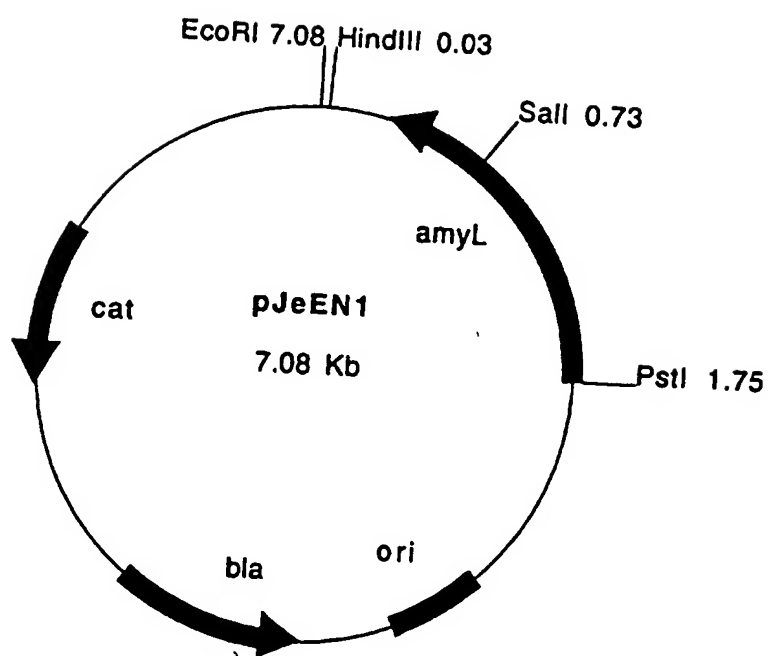


Fig. 10

1
INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

A. CLASSIFICATION OF SUBJECT MATTER

IPC6: C12N 9/28, C12N 15/56

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC6: C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPI, CA, MEDLINE, BIOSIS

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	Dialog Information Services, File 5, BIOSIS PREVIEWS, Dialog accession no. 11619266, BIOSIS no. 98219266, Machius M et al: "Crystal structure of calcium-depleted Bacillus licheni- formis alpha-amylase at 2.2 A resolution", & Journal of Molecular Biology 246 (4). 1995. 545-559	1-17
	--	
X	Dialog Information Services, file 155, MEDLINE, Dialog accession no. 08974640, MEDLINE accession no. 94289640, Svensson B: "Protein engineering in the alpha-amylase family: catalytic mechanism, substrate specificity, and stability", & Plant Mol Biol (NETHERLANDS) May 1994, 25 (2) p141-57	1-17
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☒ Further documents are listed in the continuation of Box C. ☒ See patent family annex.

- | | |
|---|--|
| <ul style="list-style-type: none"> * Special categories of cited documents: "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document but published on or after the international filing date "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "O" document referring to an oral disclosure, use, exhibition or other means "P" document published prior to the international filing date but later than the priority date claimed | <ul style="list-style-type: none"> "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention "X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art "&" document member of the same patent family |
|---|--|

Date of the actual completion of the international search

5 July 1996

Name and mailing address of the ISA:
Swedish Patent Office
Box 5055, S-102 42 STOCKHOLM
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Date of mailing of the international search report

05 -07- 1996

Authorized officer

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Telephone No. +46 8 782 25 00

The invention claimed relates to a method of constructing alpha-amylase variants with predetermined properties by comparing the three-dimensional structures of enzymes. The claims also include many alpha-amylase variants.

"A search for a special technical feature" as mentioned in PCT Rule 13.2 among the independent claims did not reveal a unifying, novel technical feature.

Accordingly, the following inventions were found:

- I Claims 1-17 focus on a method of constructing alpha-amylase variants by comparing the three-dimensional structure of a parent enzyme (Ternamyl-like alpha-amylase) with another enzyme e.g. mammalian or fungal alpha-amylases. The differences in structure are compared with the differences in function, whereafter new variants with new predictable characteristics are produced.
- II Claims 45-46 directed to a alpha-amylase variant that has decreased Ca^{2+} dependency,
- III Claim 47 directed to a alpha-amylase variant that exhibits higher activity below the pH-optimum than the parent enzyme.
- IV Claim 48 directed to a alpha-amylase variant having an increased thermostability and/or altered temperature optimum.
- V Claim 50 directed to a variant having reduced capability of cleaving an oligo-saccharide substrate close to its branching point.

Due to the complex construction of the claims and the fact that the search so far has not covered all aspects of the invention, it may be that further non-unity remarks can appear. If further searches are done, references might appear which will give further a posteriori non-unity remarks.

Therefore, the search has been restricted to the first invention.

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Claims 18-43 are directed to a number of different variants that are composed of several inventions. They are, however, so complex and broad that no meaningful search can be done, especially as no special characteristic is linked to the groups of variants. It is for example unlikely that claim 18 concerns one invention. It is not believable that a change in any amino acid in one fragment for one/or none of the amino acids in a fragment of another enzyme gives an enzyme with the same new and valuable characteristic. The formulation of claims 18-43 is so complicated because of all the different combinations of amino acid substitutions.

Thus they do not comply with Art. 6. PCT prescribing that claims shall be clear and concise.

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	Dialog Information Services, file 155, MEDLINE. Dialog accession no. 08958150, MEDLINE accession no. 94273150, Nakatani H et al: "Effect of modifying histidine residues on the action of Bacillus amylo- liquefaciens and barley-malt alpha-amylases", & Carbohydr Res (NETHERLANDS) Apr 16 1994, 257 (1) p 155-61	1-17
Y	--	45-46
X	J. MED. BIOL., Volume 229, 1993, C. Chang et al, "Crystallization and Preliminary X-ray Crystallographic Analysis of alpha-Amylase from Bacillus subtilis" page 235 - page 238	1-17
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A	WO 9100343 A2 (GIST-BROCADES N.V.), 10 January 1991 (10.01.91)	1-17
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A	EP 0410498 A2 (GIST-BROCADES N.V.), 30 January 1991 (30.01.91)	1-17
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A	JOURNAL OF BACTERIOLOGY, Volume 166, No 2, May 1986, G. L. Gray et al, "Structural Genes Encoding the Thermophilic alpha-Amylases of Bacillus stearothermophilus and Bacillus licheniformis" page 635 - page 643	1-17
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P,X	WO 9535382 A2 (GISTBROCADES B.V.), 28 December 1995 (28.12.95), claims 1-2, abstract	45-46
	--	
Y	WO 9418314 A1 (GENENCOR INTERNATIONAL), 18 August 1994 (18.08.94)	45-46
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INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	Chemical Abstracts, Volume 108, No 11, 14 March 1988 (14.03.88), (Columbus, Ohio, USA), Buisson, G. et al, "Three dimensional structure of porcine pancreatic alpha-amylase at 2.9 Å resolution. Role of calcium in structure and activity", page 325, THE ABSTRACT No 90927h, EMBO J. 1987, 6 (13), 3909-3916 --	45-46
Y	Chemical Abstracts, Volume 112, No 15, 9 April 1990 (09.04.90), (Columbus, Ohio, USA), Vihinen, Mauno et al, "Site-directed mutagenesis of a thermostable alpha-amylase from Bacillus stearothermophilus: putative role of three conserved residues", page 347, THE ABSTRACT No 135178r, J. Biochem 1990, 107 (2), 267-272 --	45-46
A	US 4600693 A (KAREN L. KINDLE ET AL), 15 July 1986 (15.07.86) --	45-46
A	Chemical Abstracts, Volume 112, No 19, 7 May 1990 (07.05.90), (Columbus, Ohio, USA), Holm, Liisa et al, "Random mutagenesis used to probe the structure and function of Bacillus stearothermophilus alpha-amylase", page 351, THE ABSTRACT No 174785f, Protein Eng. 1990, 3 (3), 181-191 -----	45-46

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK96/00057

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

see next sheet

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see next sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☒ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
Claims 1-17 directed to a method of constructing alpha-amylase variants
and claims 45-46 directed to an alpha-amylase.
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐

The additional search fees were accompanied by the applicant's protest.

☒

No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT
Information on patent family members

01/04/96

International application No.

PCT/DK 96/00057

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO-A2- 9100343	10/01/91	AU-B, B- 629959 AU-A- 5939790 CA-A- 2032518 EP-A, A, A 0409299 JP-T- 4500609	15/10/92 17/01/91 30/12/90 23/01/91 06/02/92
EP-A2- 0410498	30/01/91	AU-B- 638263 AU-A- 5953890 CA-A- 2030554 CN-A- 1050220 JP-T- 4500756 US-A- 5364782 WO-A, A, A 9100353	24/06/93 17/01/91 30/12/90 27/03/91 13/02/92 15/11/94 10/01/91
WO-A2- 9535382	28/12/95	NONE	
WO-A1- 9418314	18/08/94	NONE	
US-A- 4600693	15/07/86	NONE	

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